A CALCULATION OF THE ENERGY BANDS OF THE GRAPHITE CRYSTAL BY MEANS OF THE TIGHT-BINDING METHOD

by

FERNANDO JOSÉ CORBATÓ

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Signature of Author. . . . Signature redacted . . . . . .
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Certified by. . . . Signature redacted . . . . . .
Thesis Supervisor

Accepted by . . . . Signature redacted . . . . . .
Chairman, Departmental Committee
on Graduate Students

Abstract

Thesis Title: A Calculation of the Energy Bands of the Graphite Crystal by means of the Tight-Binding Method

Author: Fernando José Corbató

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The graphite crystal is approximated by a two-dimensional hexagonal lattice of carbon atoms. One-electron wave functions of appropriate translational symmetry are formed by making Bloch waves from the 1s, 2s, 2px, 2py, and 2pz Hartree-Fock atomic orbitals of carbon. The crystal potential is taken to be a superposition of spherically symmetric atomic potentials formed from the effective nuclear charge function of atomic carbon. From the usual variational principle, the energy bands (energy values as a function of the Bloch wave vector) are given by the solution of an 8 by 8 secular equation formed from the σ states which are symmetric in the plane of the graphite sheet and a 2 by 2 secular equation formed from the π states which are antisymmetric in the plane of the graphite sheet. The secular equation matrix elements, besides being dependent on the wave vector, require one-electron two- and three-center integrals formed from the atomic orbitals and the atomic potential. The two-center integrals are evaluated up to the ninth neighbor distances and the three-center integrals are evaluated up to the fourth neighbor distances. The secular equations are solved for 25 representative wave vectors.

The resultant one-electron energy bands show σ bands which cross over parts of the π bands. However, there is an energy gap in the σ bands which encloses the Fermi level in the π bands. Thus there is support for the usual approximation of only considering the π states in calculations of the conduction properties of three-dimensional graphite. In addition the width of the valence bands is found to be in good agreement with the experimental measurement by Chalkin.

The energy bands are also examined with respect to simplifying approximations. The inclusion of three-center integrals and of the 1s Bloch waves is found to be necessary. The π bands are stable when higher than third neighbor distance two-center integrals are neglected and the σ bands are essentially stable when higher than fifth neighbor distance two-center integrals are neglected.

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Comparison is made with a graphite energy band calculation by Lomer. It is concluded that his energy bands, which differ from the present result, can only be considered qualitatively since an insufficient number of higher neighbor distance integrals were used.

Thesis Supervisor: John C. Slater

Title: Institute Professor; Harry B. Higgins Professor of the Solid State

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Chapter 1

Introduction

The present work describes a calculation of the energy bands of a simplified graphite crystal by means of the tight-binding method. The structure of the real graphite crystal is that of carbon atoms hexagonally arranged in layers, (nearest-neighbor distance: 1.42 A°) which are stacked with a fairly large interlayer distance (3.35 A°). It is generally assumed that the interlayer binding energy of graphite is much weaker than the intralayer binding energy, a result supported by the ease of formation of stacking faults in observed crystals[1]. This qualitative behavior is associated with tightly bound intralayer electronic states and loosely bound interlayer electronic states. One approach to describing these states is to make up approximate electronic crystal wave functions as linear combinations of atomic orbitals.

In analogy to the general theory of molecular binding in organic molecules, the crystal wave functions (called π states) which are made up of the 2p atomic orbitals with nodal planes coincident with the graphite hexagonal sheets are then assigned the major share of the interlayer binding. Correspondingly, the crystal wave functions (called σ states) made up of the remaining two 2p orbitals and the 1s and 2s orbitals are said to give rise to major part of the intralayer binding of graphite. This description is the essence of the well-known tight-binding method or Bloch method[2] when it is further assumed that the crystal electronic states can be considered as independently occupied such that the crystal electronic eigenfunctions are one-electron functions governed by an one-electron effective Hamiltonian operator.

The first tight-binding calculation of three-dimensional graphite energy bands was made by Wallace[3] in 1947. He assumed that the energies of the σ and π states were sufficiently separated to allow neglect of the σ states. This assumption, however, had only a qualitative justification but has been the basis of most of the subsequent calculations of graphite energy bands such as the recent work of Johnston[4]. An exception to this is the essentially qualitative and empirical discussion made by Coulson and Taylor[5] of the graphite σ and π energy bands wherein they show the possible importance of the σ states. In addition, a calculation of the energy bands of a single two-dimensional graphite layer which included both σ and π states has been recently made by Lomer[6]. However, as will be seen in the concluding chapter an approximation was made in Lomer's work such that his results must be interpreted as qualitative ones.

The present work is an attempt to bridge the gap between the qualitative energy band treatments and the rigorous energy band treatments which are extremely difficult. In particular, as in Lomer's calculation, a single two-dimensional graphite layer was taken to represent a graphite crystal. However, in contrast to Lomer's work, no recourse has been made to empirical values and the stability of the final solution with respect to the various possible mathematical approximations has been established.

Chapter 2

Theory and Formulation

Section a: Energy Bands and the Tight-Binding Method

The theory of the tight-binding method was first formulated by Bloch[7], is comprehensively described in the text by Seitz[2], and has been recently reexamined by Slater and Koster[8]. In this section, the essential theory of the method given in these references will be briefly reviewed in the interest of completeness.

The basic principle of the tight-binding method is to approach the problem of a crystal by means of a one-electron approximation wherein the one-electron crystal wave functions are taken to be linear combinations of atomic orbitals (usually abbreviated: AO's) denoted by ψ. These linear combinations of atomic orbitals are restricted, however, by virtue of the translational symmetry of a crystal. In particular, such linear combinations must also be eigenfunctions of a translation operator T, representing a translation $\vec{R}_\ell$ which takes the crystal lattice into itself. This is because the translation operator commutes with the usual one-electron Hamiltonian operator

$$\mathcal{H}(\vec{r}) = -\tfrac{1}{2}\nabla^2 - \mathcal{V}(\vec{r}) \qquad (2\text{-}1)$$

where $\mathcal{V}(\vec{r})$ is an effective crystal potential function which has the same symmetry as the crystal lattice. (Unless otherwise stated, atomic units are used where the unit of length is the first Bohr radius and the unit of energy is two Rydbergs; the sign of the potential term in eq. 2-1 is assumed for convenience.) To consider in an orderly fashion a crystal which is infinite in size, the customary periodic boundary conditions are used; the infinite crystal is taken to be made up of an infinite number of identical N-unit cell sub-crystals. The formalism of letting N approach infinity then systematically yields the properties of the infinite crystal. Under these conditions, the appropriate linear combinations, called Bloch waves, are

$$\Psi_i(\vec{k},\vec{r}) = \frac{1}{\sqrt{N}} \sum_{\vec{R}_n} e^{i\vec{k}\cdot\vec{R}_n} \psi_i(\vec{r}-\vec{R}_n) \qquad (2\text{-}2)$$

where the sum is over the lattice vectors to each of the N unit cells of the crystal lattice and the eigenvalue of the translation operator T is $e^{i\vec{k}\cdot\vec{R}_\ell}$.

An immediate but important result is that matrix elements taken between Bloch waves of different wave vectors are zero for operators such as the one-electron Hamiltonian which are invariant under the translations T which take the crystal into itself. This follows quickly from the fact that the matrix element integral is taken over all space, and hence the value of the integral is invariant to any translation of the integrand coordinates and in particular to those translations T. Thus the equation

$$\begin{aligned} O_{ij} &= \int \Psi_i^*(\vec{k},\vec{r})\, O(\vec{r})\, \Psi_j(\vec{k}',\vec{r})\, d\tau \\ &= \int [T\Psi_i^*(\vec{k},\vec{r})][T O(\vec{r})][T\Psi_j(\vec{k}',\vec{r})]\, d\tau = e^{i(\vec{k}'-\vec{k})\cdot\vec{R}_\ell}\, O_{ij} \qquad (2\text{-}3) \end{aligned}$$

allows one to conclude that O_{ij} is zero unless $\vec{k} = \vec{k}'$.

Consequently, just as the wave vector $\vec{k}$ characterizes the translational eigenvalues, it can be used to characterize the Hamiltonian eigenvalues. For this purpose it is convenient to define a reciprocal lattice. Thus if the vectors $\vec{R}_n$ are linear combinations with integral coefficients of the primitive translation vectors $\vec{a}_i$ which define the crystal lattice unit cell, then the equations

$$\vec{a}_i \cdot \vec{b}_j = \delta_{ij} \qquad (2\text{-}4)$$

where i and j take on as many values as there are crystal dimensions, define the $\vec{b}_i$ which are the primitive translations of the reciprocal lattice unit cell. As will soon be seen, the reciprocal lattice vectors are the natural basis with which to express the wave vector $\vec{k}$.

In order to explore further the usefulness of the reciprocal lattice, the following definitions are made:

$$\vec{R}_n = \sum_i R_{ni}\,\vec{a}_i \quad , \quad R_{ni} \text{ integral} \tag{2-5a}$$

$$\vec{K}_\ell = 2\pi \sum_i K_{\ell i}\,\vec{b}_i , \quad K_{\ell i} \text{ integral} \tag{2-5b}$$

$$\vec{k} = 2\pi \sum_i k_i\,\vec{b}_i , \quad k_i \text{ all values} \tag{2-5c}$$

Then it is clear that for any wave vector $\vec{k}$, one may choose a $\vec{K}_j$ such that $\vec{k} = \vec{k}' + \vec{K}_j$ where $|\vec{k}'|$ is less than any of the non-zero $|\vec{K}_\ell|$. However, because of the relation

$$e^{i\vec{k}\cdot\vec{R}_\ell} = e^{i(\vec{k}'+\vec{K}_j)\cdot\vec{R}_\ell} = e^{i\vec{k}'\cdot\vec{R}_\ell} \tag{2-6}$$

which results from the definition of the reciprocal lattice vectors $\vec{b}_i$, it is clear that the Bloch waves for $\vec{k}$ and $\vec{k}'$ are identical so that the two values of the wave vector can be used interchangeably. Thus the eigenvalues and eigenfunctions of a spatial operator $O(\vec{r})$ are invariant in the reciprocal lattice under translations $\vec{K}_\ell$.

It is just this translational property in the reciprocal lattice which allows one to define polyhedral surfaces in the reciprocal lattice which form concentric zones about $\vec{K}_\ell = 0$ such that each zone contains a set of wave vectors associated with one set of the wave vector dependent eigenvalues of a spatial operator. These zones are called Brillouin zones. When one restricts the wave vectors to values lying within the first zone about $\vec{K}_\ell = 0$, the convention is to call this set of vectors the "reduced" wave vectors and all subsequent references in this work will be to these reduced vectors. This is in contrast to the other convention often used with plane wave approximations to the eigenfunctions where as a function of the wave vector the lowest eigenvalues are associated with the first Brillouin zone, the next highest eigenvalues with the second Brilloin zone, etc. A particularly simple way of obtaining the polyhedral surface enclosing the first Brillouin zone is to construct perpendicularly bisecting planes through the lines between $\vec{K}_\ell = 0$ and all the other $\vec{K}_\ell$ points in the reciprocal lattice; the resultant innermost envelope about $\vec{K}_\ell = 0$ then encloses the first Brillouin zone.

Having established the form of the approximate one-electron eigenfunctions, the usual variational procedure can be applied. Thus the best crystal eigenfunctions are taken as a linear combination of M Bloch waves with the same wave vector

$$\Phi_\ell(\vec{k},\vec{r}) = \sum_{i=1}^{M} C_{i\ell}(\vec{k})\,\Psi_i(\vec{k},\vec{r}) \tag{2-7}$$

where the coefficients are determined by minimizing the stationary expectation value of the Hamiltonian operator

$$E_\ell(\vec{k}) = \frac{\int \Phi_\ell^*(\vec{k},\vec{r})\,\mathcal{H}(\vec{r})\,\Phi_\ell(\vec{k},\vec{r})\,d\tau}{\int \Phi_\ell^*(\vec{k},\vec{r})\,\Phi_\ell(\vec{k},\vec{r})\,d\tau} \tag{2-8}$$

with respect to the coefficients $C_{i\ell}$. Using the Hermitian property of the Hamiltonian, the variation leads to the secular equation

$$\sum_{j=1}^{M} \mathcal{H}_{ij}(\vec{k})\, C_{j\ell}(\vec{k}) = E_\ell(\vec{k}) \sum_{j=1}^{M} \mathcal{S}_{ij}(\vec{k})\, C_{j\ell}(\vec{k}) \qquad (2\text{-}9)$$

with

$$\mathcal{H}_{ij}(\vec{k}) = \int \Psi_i^*(\vec{k},\vec{r})\, \mathcal{H}(\vec{r})\, \Psi_j(\vec{k},\vec{r})\, dr$$

$$\mathcal{S}_{ij}(\vec{k}) = \int \Psi_i^*(\vec{k},\vec{r})\, \Psi_j(\vec{k},\vec{r})\, dr$$

which for a fixed value of the wave vector has M solutions $\ell = 1, 2, \ldots M$. Considered as continuous functions of the wave vector $\vec{k}$, these Hamiltonian eigenvalues are called energy bands. The secular equation 2-9, which is more general than the usual type because of the nonorthogonality of the Bloch waves, can be solved by matrix techniques which are described in Appendix B.

A further property of the energy bands obtained by the solution of the secular equation results from additional non-translational symmetry of the Hamiltonian operator. In particular, the atomic orbitals used to form the various Bloch waves can be grouped into sets of basis functions which transform into each other under the application of the crystal symmetry operators. It will now be shown that when the Bloch waves used in the variational procedure are made up of all the atomic orbitals in a given set of basis functions, the eigenvalues resulting from the variational procedure will be invariant under the application of the crystal symmetry operators to the wave vector. Thus if the symmetry operators are designated by Γ, the Bloch waves of wave vector $\Gamma\vec{k}$ are

$$\Psi_i(\Gamma\vec{k},\vec{r}) = \frac{1}{\sqrt{N}}\sum_{\vec{R}_n} e^{i\Gamma\vec{k}\cdot\vec{R}_n}\,\psi_i(\vec{r}-\vec{R}_n) \qquad (2\text{-}10)$$

$$= \frac{1}{\sqrt{N}}\sum_{\vec{R}_n} e^{i\vec{k}\cdot\Gamma^{-1}\vec{R}_n}\,\psi_i(\vec{r}-\vec{R}_n)$$

$$= \frac{1}{\sqrt{N}}\sum_{\vec{R}_n} e^{i\vec{k}\cdot\Gamma^{-1}\vec{R}_n}\,\Gamma\psi_i(\Gamma^{-1}\vec{r}-\Gamma^{-1}\vec{R}_n)$$

After relabeling the sum one obtains

$$\Psi_i(\Gamma\vec{k},\vec{r}) = \frac{1}{\sqrt{N}}\sum_{\vec{R}_n} e^{i\vec{k}\cdot\vec{R}_n}\sum_{i'}\Gamma_{ii'}\psi_{i'}(\Gamma^{-1}\vec{r}-\vec{R}_n) = \sum_{i'}\Gamma_{ii'}\Psi_{i'}(\vec{k},\Gamma^{-1}\vec{r}) \qquad (2\text{-}11)$$

where the $\Gamma_{ii'}$ are the unitary matrix elements describing the transformation effected on the atomic orbital by the symmetry operator. Now if $O(\vec{r})$ is an operator having the same symmetry as the Hamiltonian operator or as the unit operator, then because of the fact that

$$O(\vec{r}) = O(\Gamma^{-1}\vec{r}) \qquad (2\text{-}12)$$

the matrix elements of O become

$$O_{ij}(\Gamma\vec{k}) = \int \Psi_i^*(\Gamma\vec{k},\vec{r})\,O(\Gamma^{-1}\vec{r})\,\Psi_j(\Gamma\vec{k},\vec{r})\,d\tau \qquad (2\text{-}13)$$

$$= \sum_{i',j'}\Gamma_{ii'}^*\,O_{i'j'}(\vec{k})\,\Gamma_{jj'}$$

The last expression is recognized however as the transformation which describes a change of the variational basis states by means of the unitary matrix $\Gamma_{ii'}$. Thus the eigenvalues of the secular equation 2-9 will be invariant with respect to the crystal symmetry operators applied to the wave vector. In a two-dimensional graphite crystal this allows one to only consider 1/12 of the first Brillouin zone.

Chapter 2

Section b: Application to a Graphite Sheet

In the preceding section, the general theory of the tight-binding method has been outlined. The present section will treat the explicit case of the graphite crystal in terms of the preceding formulation. The graphite crystal structure is well-known and consists of hexagonal layers of closely packed carbon atoms (nearest-neighbor distance: 1.42 A°) which are stacked with a fairly large interplane distance of 3.35A° . The stacking arrangement of the layers can be of two forms designated as ABAB... or ABCABC... . Experimental evidence indicates that the most perfect crystals are of the ABAB... form whereas crystals which are grown from carbon blacks usually are mixtures which approach the ABAB... form as the crystal size increases[1]. Thus it seems clear from this evidence and the large interplane distance that the interlayer binding is not strong. One would hope then that a two-dimensional model for graphite would have considerable physical significance, especially for those one-electron wave functions which describe the intraplane binding. The usual designation is to call the latter σ states, corresponding to the Bloch waves constructed out of the 1s, 2s, and two 2p atomic orbitals which are symmetric on reflection through the hexagonal plane. To the same approximate separation of effects, the Bloch waves constructed out of the 2p atomic orbitals which are anti-symmetric on reflection through the hexagonal plane are called π states and are associated with the interplane binding. The

σ and π designations are only rigorous symmetry designations however in the single-plane approximation to graphite since in a true three-dimensional graphite crystal the reflection symmetries no longer hold. The present calculation is based on the two-dimensional single-plane approximation to graphite since the computational difficulties of the three-dimensional crystal are considerably greater. Thus, fairly good signiifcance can be attached to the results arising from the σ states and only approximate validity can be given to the results of the π states. For comparison the various neighbor distances are given in table 2-1 and figure 2-1.

Table 2-1

Lattice Neighbor Distances of Two-Dimensional Graphite

Neighbor	Distance in Atomic Units
0	0
1	2.6845206
2	4.6497261
3	5.3690412
4	7.1025739
5	8.0535617
6	9.2994521
7	9.6791766
8	10.7380823
9	11.7015539

In fig. 2-2 is shown a diagram of two-dimensional graphite where the vectors $\vec{a}_1$ and $\vec{a}_2$ are the primitive translation vectors of the lattice and define the lozenge-shaped unit cell

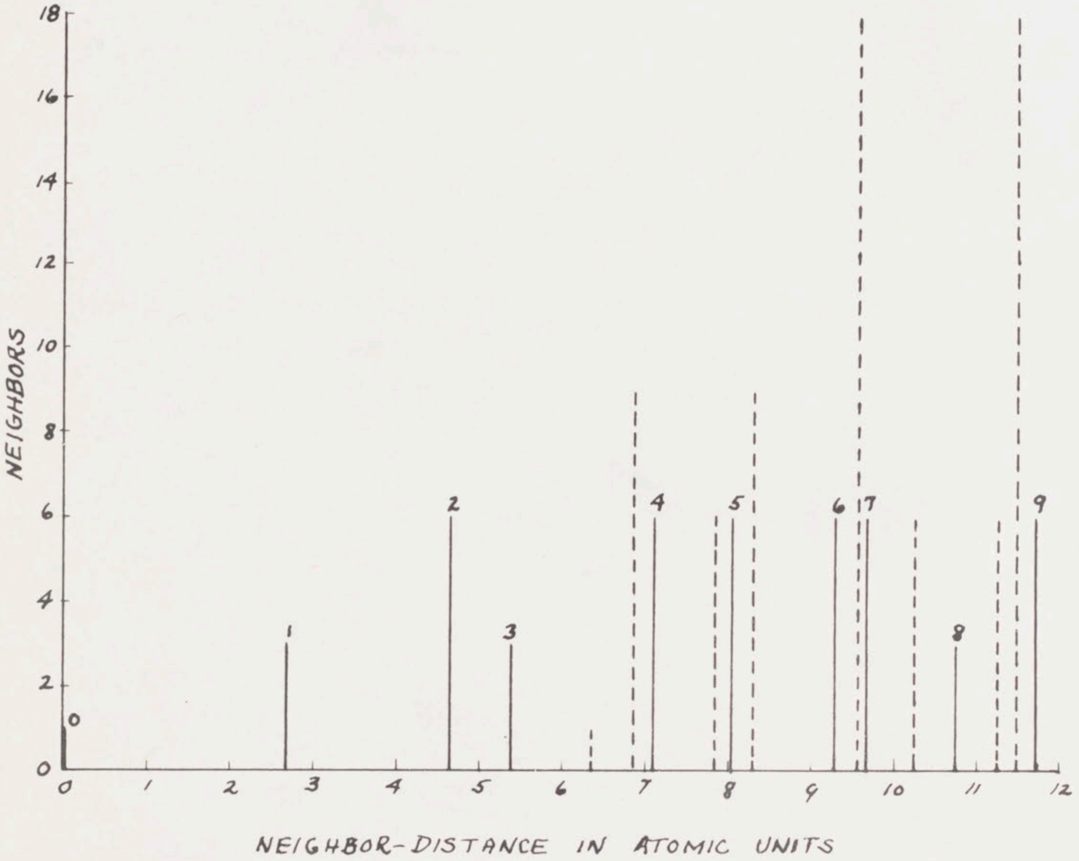


Fig. 2-1

Neighbors of Two-Dimensional Graphite

(Dotted lines give distances of comparative number of additional neighbors in three-dimensional graphite.)

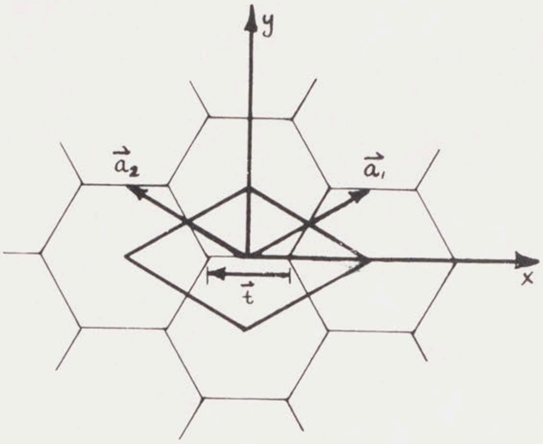


Fig. 2-2

Two-Dimensional Graphite Space Lattice Unit Cell

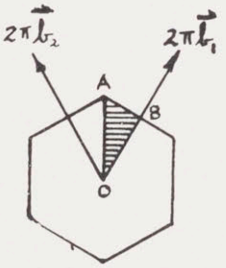


Fig. 2-3

Two-Dimensional Graphite Reciprocal Lattice Unit Cell which includes two carbon atom lattice sites. The auxiliary vector $\vec{t} = \frac{1}{3}(-\vec{a}_1 + \vec{a}_2)$ is introduced for later convenience. The corresponding two-dimensional reciprocal lattice is shown in fig. 2-3, where the vectors $\vec{b}_1$ and $\vec{b}_2$ are the primitive translations of the reciprocal lattice. The hexagon outlines the first Brillouin zone and the shaded triangle represents that smallest area of the zone from which the remaining zone energy eigenvalues may be determined by the symmetry of the Brillouin zone.

The fact that there are two carbon atoms per unit cell of the space lattice requires that the definition of the Bloch waves of the preceding section be extended. The obvious procedure is to construct Bloch waves out of atomic orbitals located on each of the two sites in the graphite unit cell. Thus each carbon atomic arbital used will give rise to two Bloch waves. It is of no particular advantage to attempt to use bonding and anti-bonding pairs of atomic orbitals to construct each Bloch wave since this concept of linear combinations of the atomic orbitals, based on maximum or minimum electronic charge overlap, continually changes as the wave vector is allowed to vary through the Brillouin zone. Furthermore, it is clear that the variational secular equation procedure used will in the end arrive at the same result.

The present calculation is based on the computation of the energy bands arising from the Bloch waves formed from the real 1s, 2s, and 2p atomic orbitals of the free carbon atom. This gives rise to eight σ states and two π states yielding an 8 by 8 and a 2 by 2 secular equation, respectively, for each value of the wave vector. Although these secular equations are capable of further factorization along the symmetry points and lines of the Brillouin zone, either by intuition or by group theoretical methods, no attempt was made to incorporate these factorizations into the computation because of the computer programming convenience in having one form of computation for all values of the wave vector.

Chapter 2

Section c: Matrix Element Formulation

Having seen that the solution of the energy band problem stems from a secular equation, the next step is to examine the matrix elements formed from the basis states of Bloch functions. For numerical solutions, it is a great simplification to have real matrix elements, whereas the previous Bloch functions will, in general, yield complex elements. However, it is clear that any unitary transformation can be made on the original basis set of functions without altering the final solution. Consequently a judicious choice of unitary transformations are applied to pairs of the Bloch functions to yield

$$\Psi_{i,q}(\vec{k},\vec{r}) = \frac{(i)^{\frac{1}{2}(1-qf_i)}}{\sqrt{2N}} \sum_{\vec{R}_n} e^{-i\vec{k}\cdot\vec{R}_n}\Big[e^{-i\vec{k}\cdot\vec{t}/2}\,\psi_i(\vec{r}-\vec{t}/2-\vec{R}_n) + qf_i p_i\, e^{i\vec{k}\cdot\vec{t}/2}\,\psi_i(\vec{r}+\vec{t}/2-\vec{R}_n)\Big] \tag{2-14}$$

where

$q = +1$ or -1

$p_i = \dfrac{\psi_i(-x,-y,-z)}{\psi_i(x,y,z)}$

$f_i = \dfrac{\psi_i(x,y,-z)}{\psi_i(x,y,z)}$

$i = nlm = 1s, 2s, 2px, 2py, 2pz$

$\vec{t} = \frac{1}{3}(-\vec{a}_1 + \vec{a}_2)$

Next computing the matrix element of the Hamiltonian operator, one finds

$$\mathcal{H}_{i,q;i',q'}(\vec{k}) = \int \Psi^{*}_{i,q}(\vec{k},\vec{r})\,\mathcal{H}(\vec{r})\,\Psi_{i',q'}(\vec{k},\vec{r})\,d\tau$$

$$= \frac{(i)^{\frac{1}{2}(qf_i - q'f_{i'})}}{2N} \sum_{\vec{R}_n} \sum_{\vec{R}_\ell} e^{-i\vec{k}\cdot(\vec{R}_n-\vec{R}_\ell)} \Big\{ \int \psi^{*}_{i}(\vec{r}-\tfrac{\vec{t}}{2}-R_\ell)\,\mathcal{H}(\vec{r})\,\psi_{i'}(\vec{r}-\tfrac{\vec{t}}{2}-R_n)\,d\tau$$

$$+ qq'f_if_{i'}\,p_ip_{i'} \int \psi^{*}_{i}(\vec{r}+\tfrac{\vec{t}}{2}-\vec{R}_\ell)\,\mathcal{H}(\vec{r})\,\psi_{i'}(\vec{r}+\tfrac{\vec{t}}{2}-\vec{R}_n)\,d\tau$$

$$+ q'f_{i'}\,p_{i'}\,e^{i\vec{k}\cdot\vec{t}} \int \psi^{*}_{i}(\vec{r}+\tfrac{\vec{t}}{2}-\vec{R}_\ell)\,\mathcal{H}(\vec{r})\,\psi_{i'}(\vec{r}-\tfrac{\vec{t}}{2}-\vec{R}_n)\,d\tau$$

$$+ qf_ip_i\,e^{-i\vec{k}\cdot\vec{t}} \int \psi^{*}_{i}(\vec{r}-\tfrac{\vec{t}}{2}-\vec{R}_\ell)\,\mathcal{H}(\vec{r})\,\psi_{i'}(\vec{r}+\tfrac{\vec{t}}{2}-\vec{R}_n)\,d\tau \Big\} \qquad (2\text{-}15)$$

It is first observed that the sum over $\vec{R}_n$ can be removed. This is done by replacing in each integral the variable $\vec{r}$ by the variable $\vec{r}+\vec{R}_n$. The vector $\vec{R}_\ell-\vec{R}_n$ then can be relabeled $\vec{R}_m$ and the sum over $\vec{R}_n$ changed to an equivalent one over $\vec{R}_m$. Then since $\mathcal{H}(\vec{r}+\vec{R}_n)=\mathcal{H}(\vec{r})$, every one of the N terms in the sum over $\vec{R}_\ell$ is the same, so that performing the sum just cancels the already present factor of $1/N$. As a further step the signs of the arguments of ψ_i and $\psi_{i'}$ in the second and fourth integrals are reversed which gives new factors of $p_ip_{i'}$. Then because of the fact that

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(-x,-y,-z)\,dx\,dy\,dz = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(x,y,z)\,dx\,dy\,dz \qquad (2\text{-}16)$$

and $\mathcal{H}(-\vec{r})=\mathcal{H}(\vec{r})$, the sign of $-\vec{r}$ can be reversed in the arguments of the second and fourth integrals. The result of the above steps is

$$\begin{aligned}\mathcal{H}_{i,q;i',q'}(\vec{k}) = \tfrac{1}{2}\,(i)^{\frac{1}{2}(qf_i - q'f_{i'})} \Big\{ & \sum_{\vec{R}_m} e^{i\vec{k}\cdot\vec{R}_m} \int \psi_i^*(\vec{r}-\vec{t}/2-\vec{R}_m)\,\mathcal{H}(\vec{r})\,\psi_{i'}(\vec{r}-\vec{t}/2)\,d\tau \\ & + \sum_{\vec{R}_m} qq'f_if_{i'}\, e^{i\vec{k}\cdot\vec{R}_m} \int \psi_i^*(\vec{r}-\vec{t}/2+\vec{R}_m)\,\mathcal{H}(\vec{r})\,\psi_{i'}(\vec{r}-\vec{t}/2)\,d\tau \\ & + \sum_{\vec{R}_m} q'f_{i'}p_{i'}\, e^{i\vec{k}\cdot(\vec{R}_m+\vec{t})} \int \psi_i^*(\vec{r}+\vec{t}/2-\vec{R}_m)\,\mathcal{H}(\vec{r})\,\psi_{i'}(\vec{r}-\vec{t}/2)\,d\tau \\ & + \sum_{\vec{R}_m} qf_ip_i\, e^{i\vec{k}\cdot(\vec{R}_m-\vec{t})} \int \psi_i^*(\vec{r}+\vec{t}/2+\vec{R}_m)\,\mathcal{H}(\vec{r})\,\psi_{i'}(\vec{r}-\vec{t}/2)\,d\tau \Big\} \end{aligned} \qquad (2-17)$$

Now because the sum over $\vec{R}_m$ is over the entire periodic lattice, $\vec{R}_m$ can be replaced by $-\vec{R}_m$ in the second and fourth sums of eq. 2-17, so that if we let a new vector $\vec{\rho}_r$ be either $\vec{R}_m$ or $\vec{R}_m+\vec{t}$ the expression can be written in the final form

$$\begin{aligned}\mathcal{H}_{i,q;i'q'}(\vec{k}) = \sum_{\vec{\rho}_r} g_{i,q;i',q'}(\vec{\rho}_r) \Big\{ & \delta(qf_i, q'f_{i'}) \cos(\vec{k}\cdot\vec{\rho}_r) \\ & + \left[1-\delta(qf_i, q'f_{i'})\right] q'f_{i'} \sin(\vec{k}\cdot\vec{\rho}_r) \Big\}\, \overline{H}_{ii'}(\vec{\rho}_r)\end{aligned}$$

where

$$g_{iq;i',q'}(\vec{\rho}_r) = \begin{cases} 1 & , \text{ if } \vec{\rho}_r = \vec{R}_m \\ qf_ip_i , & \text{ if } \vec{\rho}_r = \vec{R}_m + \vec{t} \end{cases}$$

$$\overline{H}_{ii'}(\vec{\rho}_r) = \int \psi_i^*(\vec{r}-\vec{t}/2-\vec{\rho}_r)\,\mathcal{H}(\vec{r})\,\psi_{i'}(\vec{r}-\vec{t}/2)\,d\tau \qquad (2-18)$$

and δ is the ordinary Kronecker delta function.

It is obvious that the matrix elements of $\mathcal{H}(\vec{r})$ are real when the basis states given by the set 2-14 are used. However, this is not the only set that will do the task. By examining the derivation of eq. 2-18 it can be seen that the only essential feature utilized was the centrosymmetric property,

$\mathcal{H}(\vec{r}) = \mathcal{H}(-\vec{r})$, so that in general one would follow the pattern of the above derivation using undetermined coefficients for the original unitary transformation applied to the Bloch functions and then by inspection determine the appropriate basis functions; if this were not possible by inspection, recourse to group-theoretical methods would be required.

In addition, the derivation of the formula for the overlap matrix elements follows precisely the same form as for the Hamiltonian matrix elements where $\bar{S}_{ii'}(\vec{\rho}_n)$ only differs from $\bar{H}_{ii'}(\vec{\rho}_n)$ in that $\mathcal{H}(\vec{r})$ is replaced by unity in the integral. This matrix element form allows relatively straightforward computer coding for automatic generation of the matrix elements as a function of $\vec{k}$.

As a final step in the analysis of the matrix elements, the integral values $\bar{H}_{ii'}(\vec{\rho}_n)$ and $\bar{S}_{ii'}(\vec{\rho}_n)$ will now be taken one step further so as to minimize the number of basic integral values required. In particular, the indices i and i′ refer to orbitals which are quantized with respect to the fixed coordinates of the lattice whereas the more elementary description is to quantize the orbitals with respect to the two-center axis of $\vec{\rho}_n$. Thus if the two-dimensional graphite sheet is taken to lie in the x-y plane, the 1s, 2s, and 2pz orbitals will be invariant under this requantization whereas the 2px and 2py orbitals will form new linear combinations. This new quantization of the orbitals about the axis of $\vec{\rho}_n$ is labeled by σ , π and $\bar{\pi}$ as shown in fig. 2-4. The corresponding integrals involving these new orbitals are given without a bar as $H_{ii'}(\vec{\rho}_n)$ and $S_{ii'}(\vec{\rho}_n)$. The transformation which is the same for the H or S integrals is given algebraically as

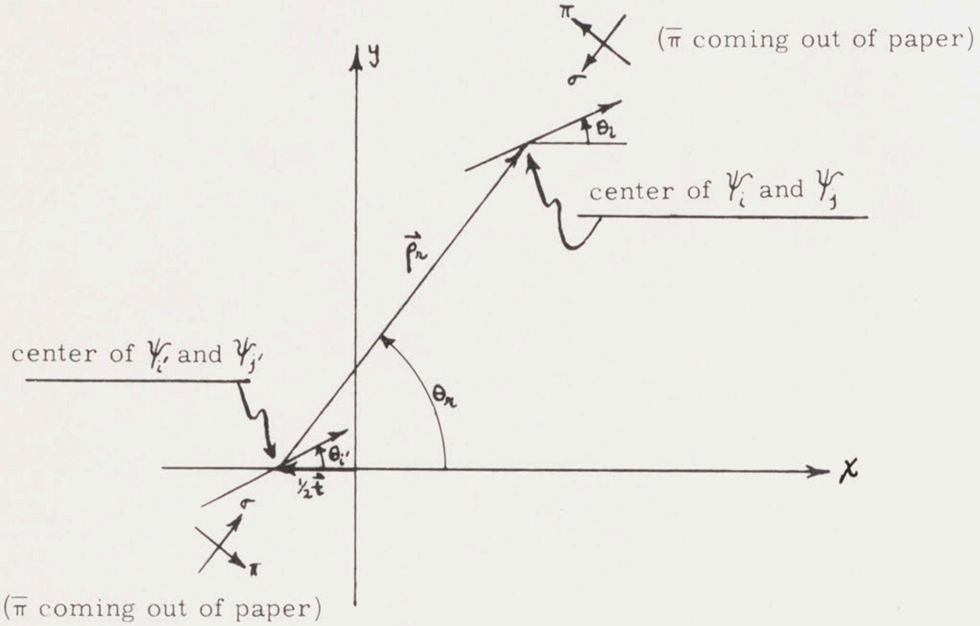


Fig. 2-4
Geometry of requantization from $\overline{M}_{ii'}(\vec{\rho}_r)$ to $M_{jj'}(\vec{\rho}_r)$ integrals, where the arrows at the centers give minus-to-plus directions of the 2p orbitals and the i, i' indices refer to 1s, 2s, 2px, 2py, 2pz orbitals and the j, j' indices refer to $1s\sigma$, $2s\sigma$, $2p\sigma$, $2p\pi$, $2p\overline{\pi}$ orbitals.

$$\overline{M}_{ii'}(\vec{\rho}_n) = \sum_j \sum_{j'} U_{ij}\, U'_{i'j'}\, M_{jj'}(\vec{\rho}_n) \qquad (2\text{-}19)$$

where using the angles designated in fig. 2-4 the transformation matrices are

$$U_{ij} = \begin{array}{c|ccccc} & j=1s & 2s & 2p\sigma & 2p\pi & 2p\bar{\pi} \\ \hline i=1s & 1 & 0 & 0 & 0 & 0 \\ 2s & 0 & 1 & 0 & 0 & 0 \\ 2px & 0 & 0 & -\cos\theta_n & -\sin\theta_n & 0 \\ 2py & 0 & 0 & -\cos(\theta_n-\pi/2) & -\sin(\theta_n-\pi/2) & 0 \\ 2pz & 0 & 0 & 0 & 0 & 1 \end{array}$$

$$U'_{i'j'} = \begin{array}{c|ccccc} & j'=1s & 2s & 2p\sigma & 2p\pi & 2p\bar{\pi} \\ \hline i'=1s & 1 & 0 & 0 & 0 & 0 \\ 2s & 0 & 1 & 0 & 0 & 0 \\ 2px & 0 & 0 & \cos\theta_n & \sin\theta_n & 0 \\ 2py & 0 & 0 & \cos(\theta_n-\pi/2) & \sin(\theta_n-\pi/2) & 0 \\ 2pz & 0 & 0 & 0 & 0 & 1 \end{array}$$

Now in the computer program used to generate the $\overline{H}_{ii'}(\vec{\rho}_n)$ and $\overline{S}_{ii'}(\vec{\rho}_n)$ from the $H_{ii'}(\vec{\rho}_n)$ and $S_{ii'}(\vec{\rho}_n)$ the following short-cuts were used to effect the above transformation. First because of the basic factorization of the secular equation into the so-called σ states and π states and the equivalent transformation properties of 1s, 2s, and 2pz states under rotation in the graphite sheet, the secular equations arising from the 2pz Bloch waves were solved separately by allowing the 2pz input data to masquerade as 2s input data. Moreover by picking special values of θ_i and $\theta_{i'}$ for the non-directional 1s and 2s functions it was possible to effect the transformation in a uniform way by means of the formula

$$
\begin{aligned}
\overline{M}_{ii'}(\vec{\rho}_r) = -\Big\{ & \cos(\theta_r-\theta_i)\cos(\theta_r-\theta_{i'})\, M_{nl\sigma,nl\sigma}(\vec{\rho}_r) \\
& + \cos(\theta_r-\theta_i)\sin(\theta_r-\theta_{i'})\, M_{nl\sigma,nl\pi}(\vec{\rho}_r) \\
& + \sin(\theta_r-\theta_i)\cos(\theta_r-\theta_{i'})\, M_{nl\pi,nl\sigma}(\vec{\rho}_r) \\
& + \sin(\theta_r-\theta_i)\cos(\theta_r-\theta_{i'})\, M_{nl\pi,nl\pi}(\vec{\rho}_r) \Big\}
\end{aligned}
\qquad (2\text{-}20)
$$

where

$\theta_i = 0$, if $i = 2px$; $\theta_{i'} = 0$, if $i' = 2px$

$\theta_i = \pi/2$, if $i = 2py$; $\theta_{i'} = \pi/2$, if $i' = 2py$

$\theta_i = \theta_r + \pi$, if $i = 1s, 2s, 2pz$; $\theta_{i'} = \theta_r$, if $i' = 1s, 2s, 2pz$

It should be clear that the requantization transformation matrices would have become more complicated if higher quantum number orbitals had been used. In fact, the machinery for systematically handling these rotations is given in Chapter 5 where the general rotation of spherical harmonics is discussed. However, this machinery was only developed towards the conclusion of this work so that in retrospect it is felt that rather than the above short cuts the more elaborate yet systematic and general matrix techniques should have been used.

The specification of input data for the secular equations is thus resolved to the basic $H_{ii'}(\vec{\rho}_r)$ and $S_{ii'}(\vec{\rho}_r)$ integrals. The Hamiltonian integrals are next separated into kinetic and potential energy terms. Thus

$$H_{ii'}(\vec{\rho}_r) = T_{ii'}(\vec{\rho}_r) - V_{ii'}(\vec{\rho}_r) \qquad (2\text{-}21)$$

where $$T_{ii'}(\vec{\rho}_n) = \int \psi_i^*(\vec{r} - \vec{t}/2 - \vec{\rho}_n)\left[-\tfrac{1}{2}\nabla^2\right]\psi_{i'}(\vec{r} - \vec{t}/2)\, d\tau$$

$$V_{ii'}(\vec{\rho}_n) = \int \psi_i^*(\vec{r} - \vec{t}/2 - \vec{\rho}_n)\left[\sum_{\vec{\rho}_a} \frac{Z_p(\vec{r} - \vec{\rho}_a)}{|\vec{r} - \vec{\rho}_a|}\right]\psi_{i'}(\vec{r} - \vec{t}/2)\, d\tau$$

and the sign convention of $V_{ii'}$ is taken for convenience.

To discuss further the computation of these integral values, it is useful to replace the vector $\vec{\rho}_n$ by the coordinate indices $\lambda\mu\nu$. The index λ will label the neighbor distance from the lattice point $\vec{r} = \vec{t}/2$ which is $\lambda\mu\nu = 000$. The index μ labels the sequence of lattice points at distance λ which occur upon counter-clockwise rotation in the first 120° - sector from the x-axis. Finally the index ν labels the 120° - sector. These coordinates are illustrated in fig. 2-5. It is first observed that the overlap and kinetic energy integrals depend only on distance. Thus

$$S_{ii'}(\lambda\mu\nu) = S_{ii'}(\lambda 00) \qquad (2\text{-}22)$$

$$T_{ii'}(\lambda\mu\nu) = T_{ii'}(\lambda 00) \qquad (2\text{-}23)$$

The computation of the latter integrals is described in Chapter 4 so that there only remains to discuss the more complicated potential integrals.

Now because of the trigonal symmetry of the graphite lattice, it can be immediately observed that

$$V_{ii'}(\lambda\mu\nu) = V_{ii'}(\lambda\mu 0) \qquad (2\text{-}24)$$

The remaining symmetry properties are not so obvious but are obtained most easily by inspection of fig. 2-5 . It is found that up to $\lambda = 9$, the following relations hold when $V_{ii'}(\lambda 10)$ exists:

$V_{ii'}(\lambda 10) = V_{ii'}(\lambda 00)$, for ii' of the form $\sigma\sigma$, $\pi\pi$, $\bar{\pi}\bar{\pi}$
with the exception of the $\lambda = 5$ case. (2-25)

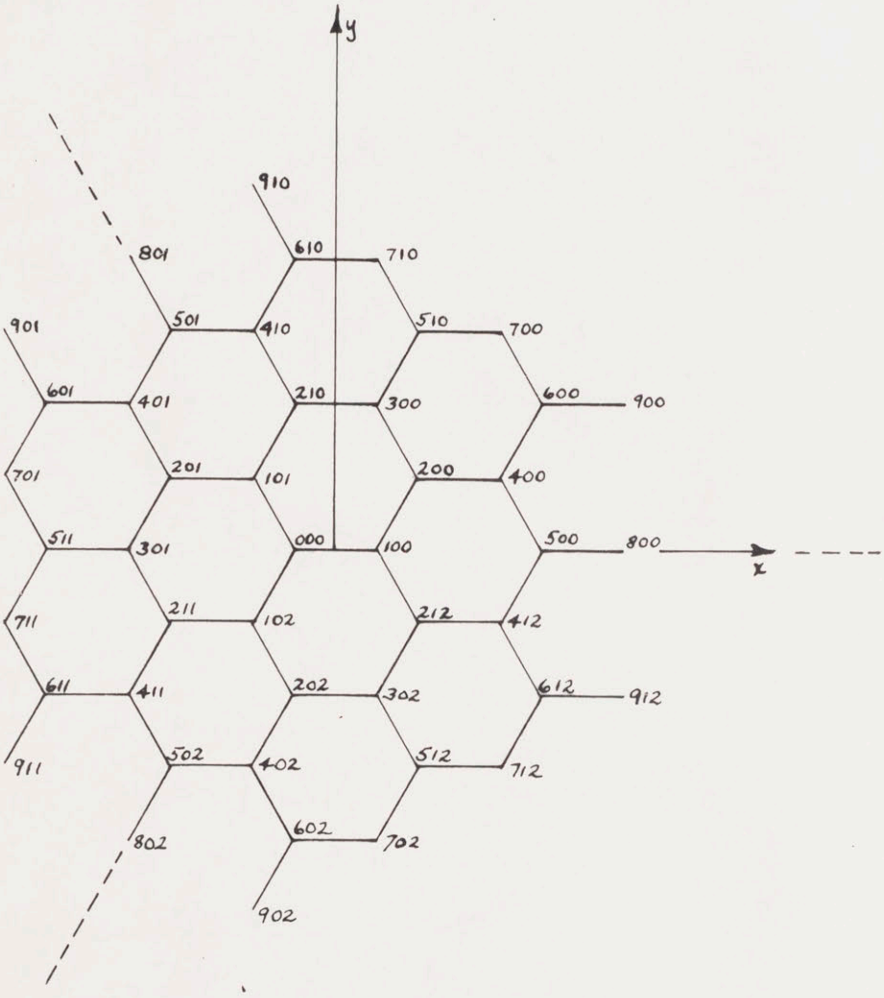


Fig. 2-5

Two-dimensional graphite neighbors in terms of the indices $\lambda\mu\nu$, where λ is the neighbor distance index, μ is the triad index, and ν is the sector index.

and $V_{ii'}(\lambda 10) = -V_{ii'}(\lambda 00)$, for ii' of the form $\sigma\pi, \pi\sigma$. (2-26)

with the special case of

$$V_{ii'}(\lambda 00) = 0, \quad \text{for the } ii' \text{ of the form } \sigma\pi, \pi\sigma \text{ and } \lambda = 0, 1, 3, 5, 8 \qquad (2\text{-}27)$$

Thus if the matrix elements of the secular equation are to be constructed from the $\lambda = 0$ to 9 components, the $V_{ii'}$ integrals arising from the following neighbor sites must be specified. $\lambda\mu\nu =$ 000, 100, 200, 300, 400, 500, 510, 600, 700, 800, 900.

Having minimized the number of basic $V_{ii'}$ integrals it remains to decompose these into the final three-center integrals. Thus

$$V_{ii'}(\lambda\mu 0) = \sum_{\lambda'\mu'\nu'} P_{ii'}(\lambda\mu 0 | \lambda'\mu'\nu') \qquad (2\text{-}28)$$

where

$$P_{ii'}(\lambda\mu 0 | \lambda'\mu'\nu') = \int \psi_i^*(\vec{r} - \vec{\rho}_{\lambda\mu 0}) \frac{Z_p(\vec{r} - \vec{\rho}_{\lambda'\mu'\nu'})}{|\vec{r} - \vec{\rho}_{\lambda'\mu'\nu'}|} \psi_{i'}(\vec{r} - \vec{\rho}_{000}) \, d\tau$$

It is the $P_{ii'}$ which are in general called three-center integrals and whose computation is discussed in Chapter 5. Finally we note that the two-center approximation, (i.e. neglect of three-center potential integrals), in this formulation, consists of making the assumption that

$$P_{ii'}(\lambda\mu 0 | \lambda'\mu'\nu') = 0 \qquad (2\text{-}29)$$

for $\lambda' \neq \lambda$ or 0, $\mu' \neq \mu$ and $\nu' \neq 0$.

Chapter 3

Choice and Fitting of Atomic Orbitals and Effective Potential

The atomic orbitals used to make up the one-electron Bloch waves were the Hartree-Fock atomic orbitals of the ground state neutral carbon ^3P configuration calculated by Jucys[9]. The 1s and 2p orbitals were each fitted by a linear combination of three corresponding analytic Slater atomic orbitals, and the noded 2s orbital was fitted by a sum of three 1s and three 2s Slater atomic orbitals. The fits were of high accuracy and were made for ease in the calculation of the many integrals. In the sense that the energy band calculation made was a one-electron approximation, it was necessary to choose an effective potential for the crystal. The crystal potential was taken to be a superposition of spherically symmetric atomic potentials. The atomic potential in turn was assumed to be the Coulombic potential arising from the effective nuclear charge function, centered on the atomic nucleus. The Z_p function for the ^3P configuration has been calculated by Freeman[10], and it was because of this convenience that the particular configuration of carbon chosen was used since it was not felt that the current knowledge of energy band solutions gave any other conclusive choice. For computational convenience, the Z_p function was also fitted, a linear combination of four exponentials being used.

The semi-automatic analytic fitting process deserves further mention since it represents a departure from the usual graphical techniques of Slater[11] or the algebraic techniques of Lowdin.[12] The process developed was an iterative one and is only suitable for use on a high-speed computer.

In particular when the radial part of a numerically tabulated Hartree-Fock atomic orbital is divided by appropriate powers of r, (or in the case of a noded 2s function by a node factor, $r_{node} - r$), the resultant numerical function is found to be exponential-like with the approximate form e^{-br}. Due to screening effects, these exponential-like functions are found to start out near $r = 0$ with a high value of b and to shift to lower values of b as r approaches infinity, the shift being empirically observed as monotonic. Thus, as is well-known, the possibility exists of approximating the numerical function by a linear combination of exponentials all with positive coefficients.

The graphical fitting method gave the motivation for the computer method which was developed. Graphically, one first plots the exponential-like function on a semi-log paper. This yields a nearly straight line with negative slope and positive second derivative. Next one approximates the fitting exponential having the lowest value of b with a straight line fit through two points of the tail region (i.e. large r). From the difference between the exponential-like function and the tail region exponential, one determines a second exponential describing the correction necessary for the inner region. In most cases, however, the inner region exponential makes a substantial contribution to the tail region so that the sum of the two fitting exponentials is too large in the tail. By using the first approximation determined for the inner region exponential, it is possible though to make a second approximation to the tail region exponential. For a two exponential fit, recycling of this process by graphical trial-and-error usually gives satisfactory consistency.

For more than two exponential fits the graphical procedure becomes somewhat complex because of the several degrees of freedom. However, because of the great iterative capacity of a computer, extending the philosophy of the graphical procedure is a feasible method. The function to be fitted is divided up into as many regions as there are to be fitting exponentials. With each of these regions a fitting exponential is assigned and two representative values of r are chosen which will serve as fitting points. The final fitting conditions will then be when each exponential at its two fitting points just equals the difference between the exponential-like function and the sum of all the other exponentials. These conditions are not a solution though since they involve knowing all the exponentials at once, whereas each condition can only be solved for one exponential.

An appropriate procedure is to first determine the exponential for each of the various regions by neglecting the effect of all the other exponentials. Thus the initial approximation to the exponential of each region is determined by two points of the exponential-like function. Next the exponential of each region is recomputed taking slight account of all the other approximate exponentials. This process of recomputation is repeatedly recycled with gradually more and more account being taken of all the other approximate exponentials. Finally when each exponential is being computed with essentially full consideration being given to all the other approximately correct exponentials, continued iteration should yield the desired self-consistent solution.

The computer process thus proceeds as follows. If the exponential-like factor of the numerically-given orbital is designated by $E^{\infty}(r)$, then for an n-exponential fit, n pairs of r_i' and r_i'' are chosen from the different regions of the function such that $r_1' > r_1'' > r_2' > r_2'' > \ldots > r_n' > r_n''$. In addition a new function is defined to be the jth approximation to $E^{\infty}(r)$.

$$E^{j}(r) \equiv \sum_{i=1}^{n} a_i^j e^{-b_i^j r} \qquad (3\text{-}1)$$

The iterative process then consists of cyclically evaluating the left-hand sides of the following pair of equations for values of i successively assuming the values 1, 2, ... n. Thus using the definition

$$D^{j}(r_i) \equiv E^{\infty}(r_i) - (1-\lambda^j)\left[\sum_{k=1}^{i-1} a_k^{j+1} e^{-b_k^{j+1} r_i} + \sum_{k=i+1}^{n} a_k^{j} e^{-b_k^{j} r_i}\right] \qquad (3\text{-}2)$$

the pair of equations are

$$b_i^{j+1} = (r_i'' - r_i')^{-1} \ln\left[\frac{D^j(r_i')}{D^j(r_i'')}\right] \tag{3-3}$$

$$a_i^{j+1} = D^j(r_i')\, e^{b_i^{j+1} r_i'} \tag{3-4}$$

where λ is an arbitrary positive constant slightly less than unity, and the initial conditions are

$$a_i^0 = b_i^0 = 0 \tag{3-5}$$

Examination of these equations reveals that as j approaches a large value J, the coupling factor, $1-\lambda^j$, approaches unity and the cyclical equations approach the 2n conditions of

$$E^J(r_i') = E^\infty(r_i') \tag{3-6}$$

and

$$E^J(r_i'') = E^\infty(r_i'') \tag{3-7}$$

Thus if λ is not too close to unity and J is large enough, the set of a_i^j and b_i^j will smoothly approach the desired parametric values.

To show algebraically the validity of eqs. 3-6 and 3-7, it is assumed that for large J, the approximate relations hold

$$a_i^{J+1} = a_i^J \tag{3-8}$$

$$b_i^{J+1} = b_i^J \tag{3-9}$$

Thus since λ^J is negligible compared to unity, eq. 3-2 becomes

$$D^J(r_i') = E^\infty(r_i') - E^J(r_i') + a_i e^{-b_i^J r_i'} \tag{3-10}$$

$$D^J(r_i'') = E^\infty(r_i'') - E^J(r_i'') + a_i e^{-b_i^J r_i''} \tag{3-11}$$

so that

$$b_i^{J+1} = (r_i'' - r_i')^{-1} \ln \left[\frac{D^J(r_i') - E^\infty(r_i') + E^J(r_i')}{D^J(r_i'') - E^\infty(r_i'') + E^J(r_i'')} \right] \tag{3-12}$$

$$a_i^{J+1} = \left[D^J(r_i') - E^\infty(r_i') + E^J(r_i') \right] e^{b_i^{J+1} r_i'} \quad . \tag{3-13}$$

Consequently the conditions

$$E^\infty(r_i) - E^J(r_i) = 0 \quad , \quad i = i', i'' \tag{3-14}$$

are self-consistent with eqs. 3-3 and 3-4.

For convenience, after convergence of the iterative fitting process is attained, the error function, $E^J(r) - E^\infty(r)$, can be automatically plotted and photographed on the computer oscilloscope camera. From the shape of the error curve, new choices of the fitting points, r_i' and r_i'' , can be made and with a few re-runs, optimization of the fit can be essentially attained. Empirically it appears that all Hartree-Fock atomic orbitals can be fitted in this manner.

The coupling factor, $1 - \lambda^j$, of eq. 3-2 deserves further comment. As a first attempt to develop the preceding iterative scheme, the coupling factor was omitted (i.e. replaced by unity). This led to a numerical "catastrophe" wherein during calculation the argument of the logarithm taken in eq. 3-3 became negative. In other words the more straight-forward cyclical equations were unstable in the sense that during the early iterations the approximate exponential fit "over bit" into the exponential-like function being fitted. Consequently, the coupling factor was introduced so as to have the effect of gradually changing over from the computation of a well-defined solution to the somewhat unstable solution of the coupled cyclical equations. In practice, for n = 3 a value of λ from .75 to .93 was used and the total number of iterations, J, required varied from 50 to 300. Figs. 3-1, 3-2 and 3-3 give plots of the Hartree-Fock radial probability functions, P(r), (r times the normalized radial factor of the atomic orbital), of the 1s, 2s, and 2p atomic orbitals which were to be fitted. (The function P (r) rather than $E^{\infty}(r)$ was used for minimizing the fitting error because of its more obvious physical significance.) Figs. 3-4, 3-5 and 3-6 give plots of the P(r) error function arising from the roughly optimum 3-exponential fitting functions. Table 3-1 gives the fitting parameters which were found including the relative coefficients of the exponentials, a_i , and the analytically renormalized coefficients which give the correct linear combination of analytic Slater atomic orbitals.

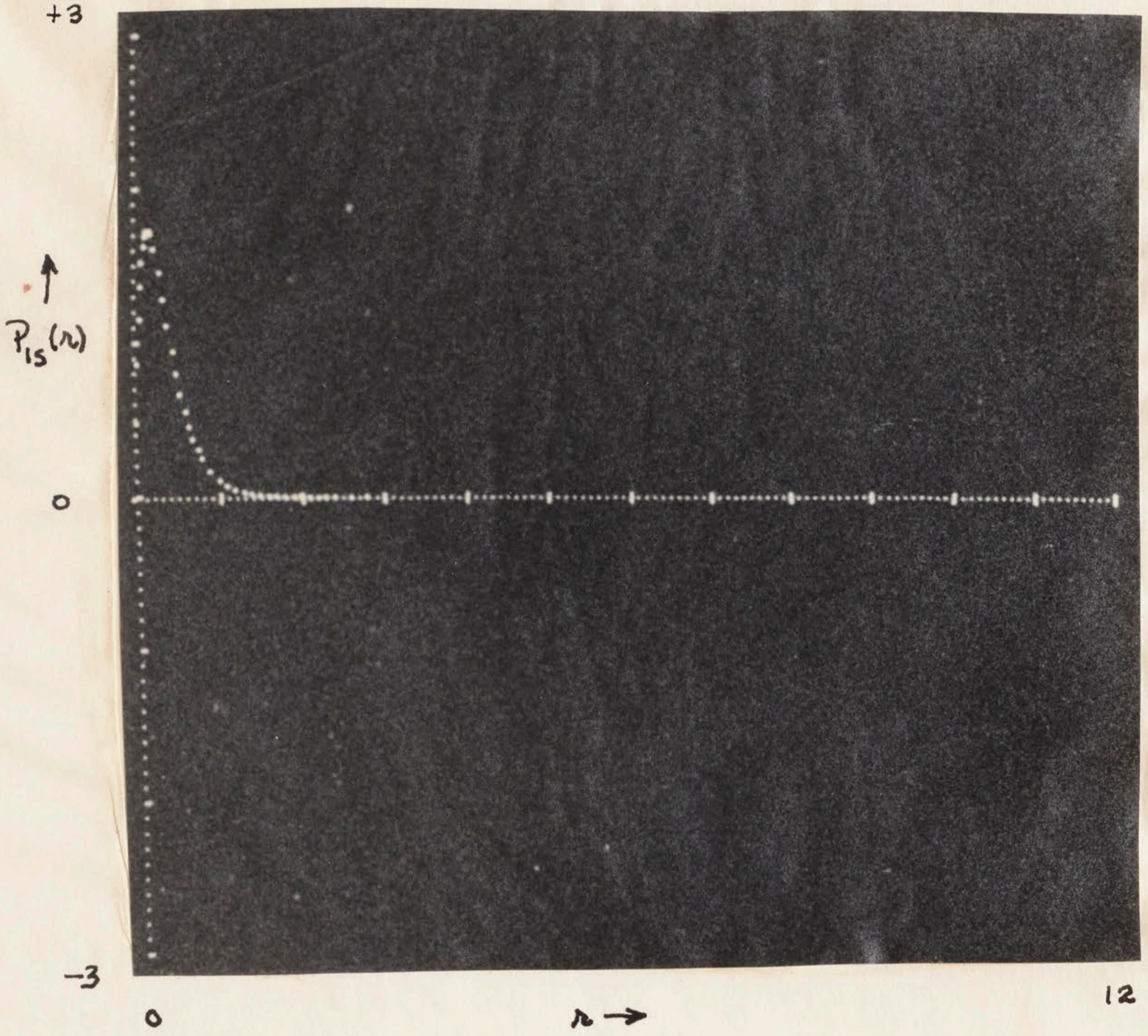


Fig. 3-1
Plot of $P_{1s}(r)$

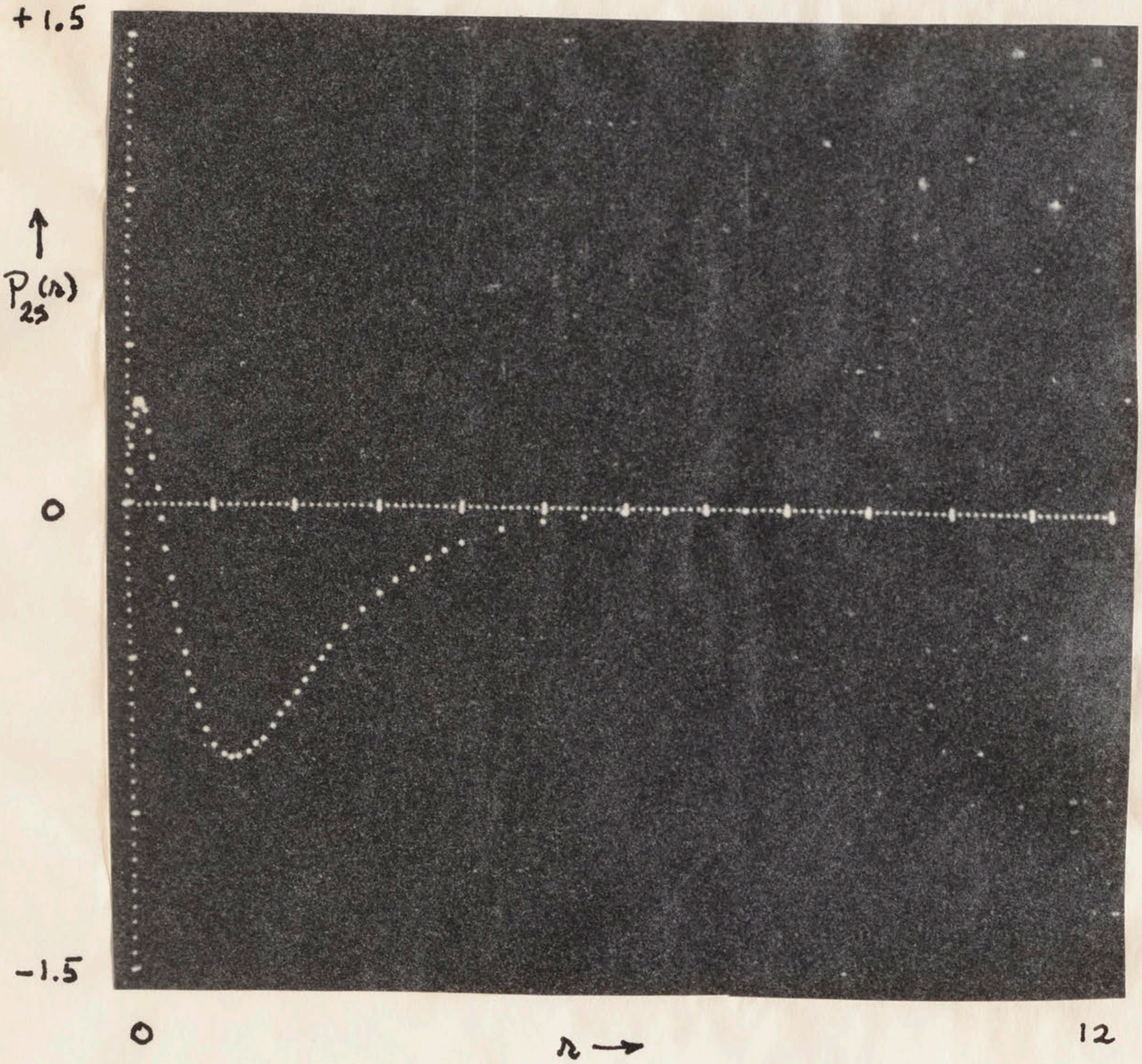


Fig. 3-2
Plot of $P_{2s}(r)$

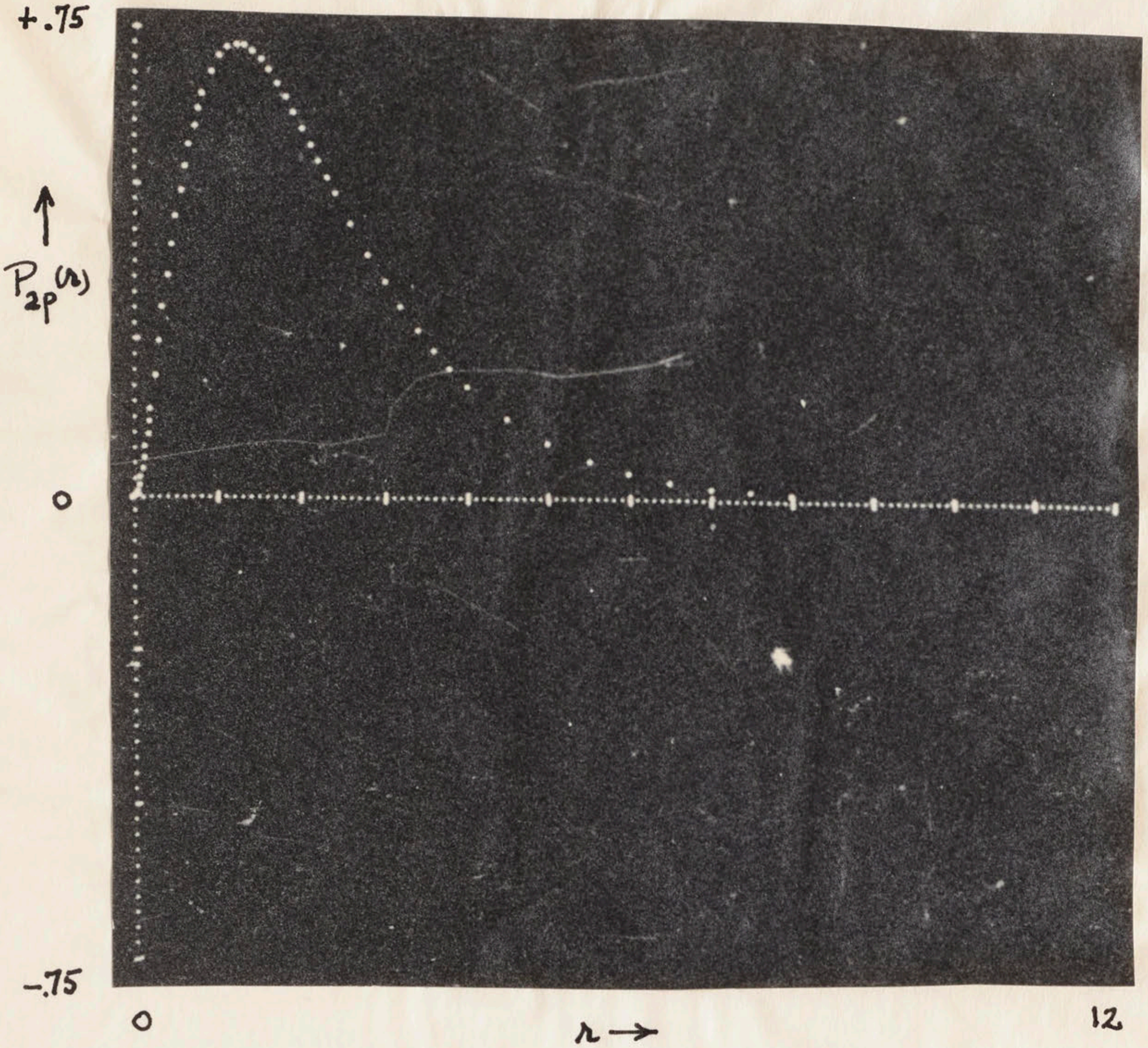


Fig. 3-3
Plot of $P_{2p}(r)$

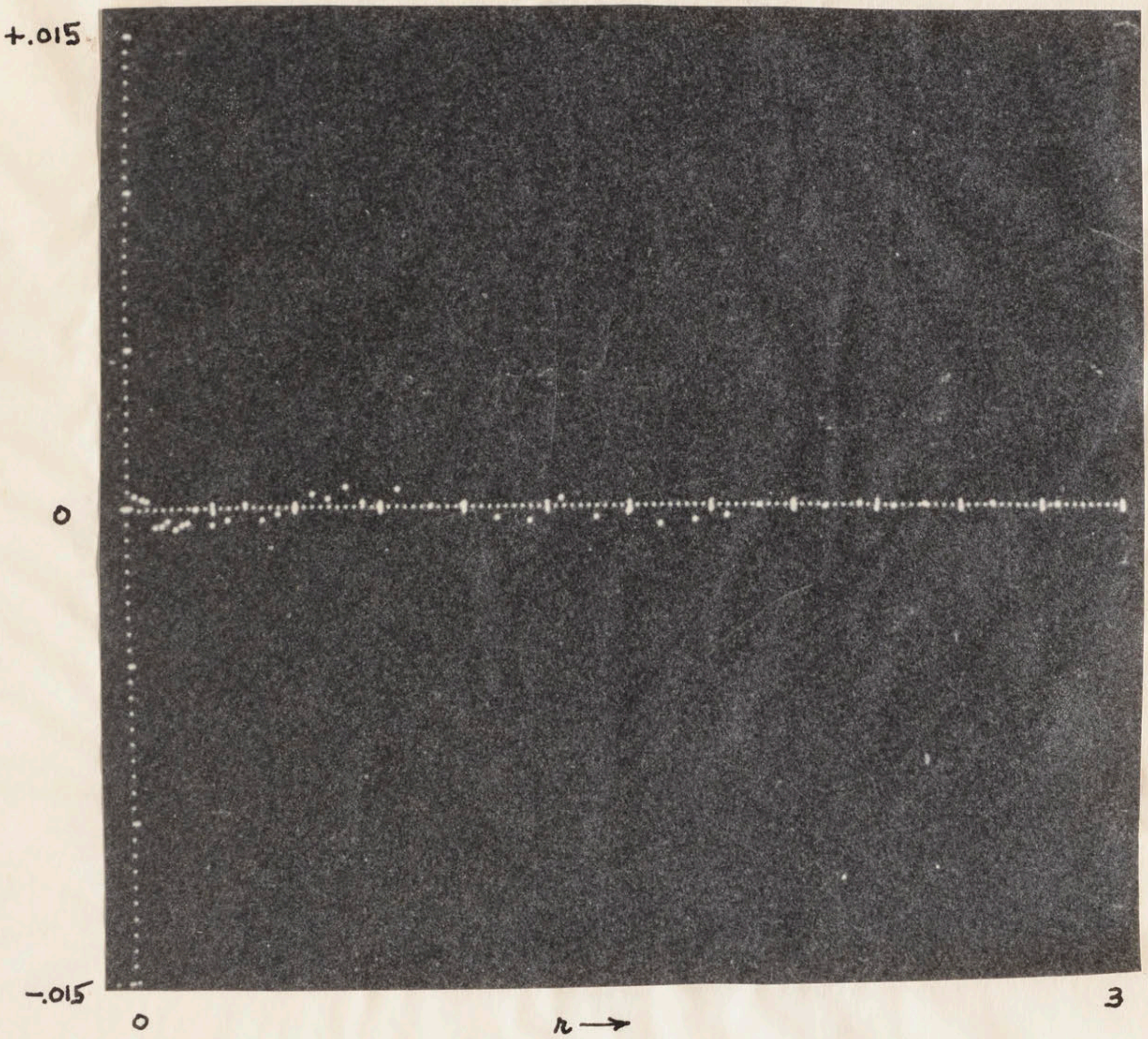


Fig 3-4
Plot of $P_{fit}(r) - P_{num}(r)$ for 1s Orbital

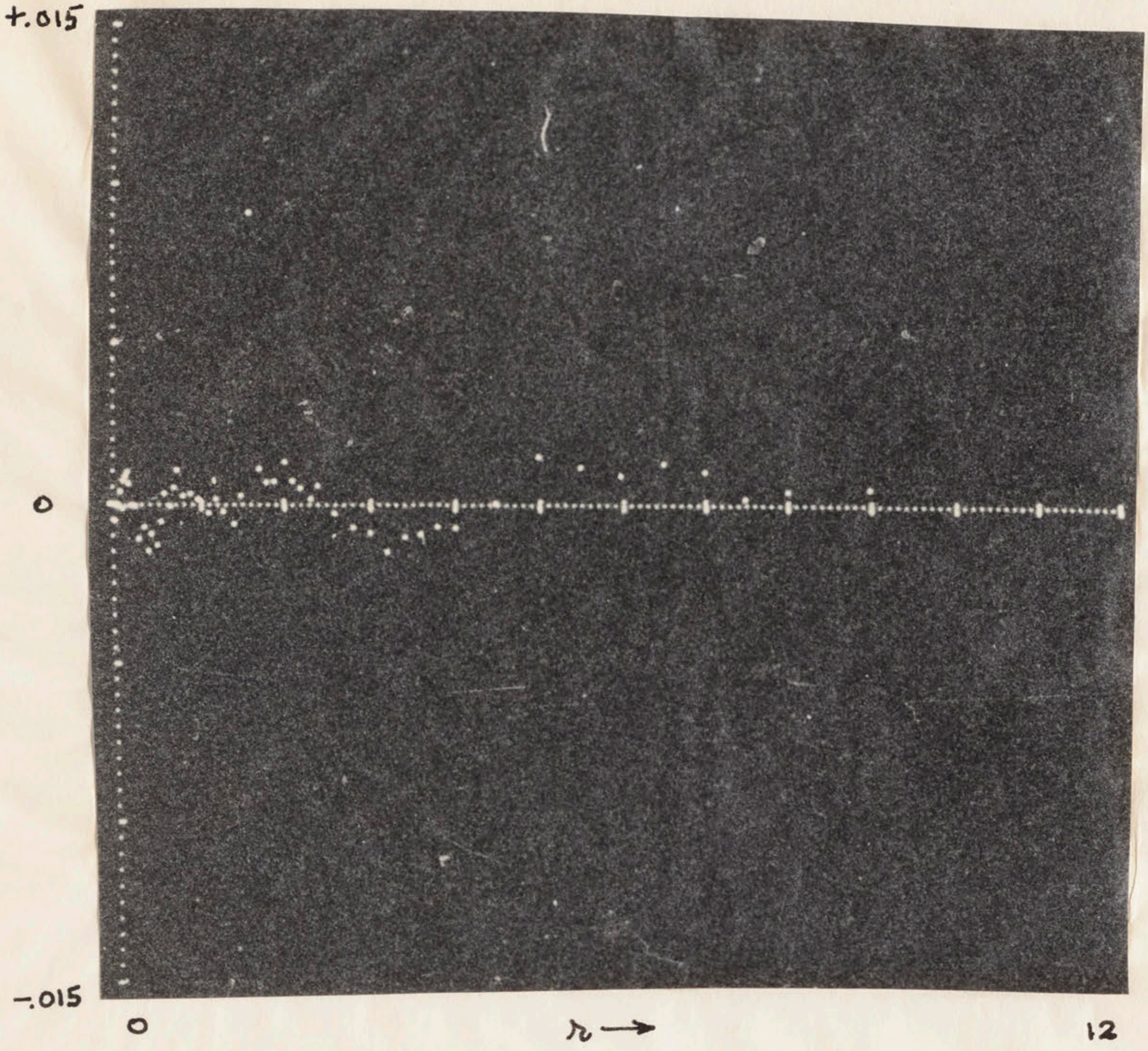


Fig. 3-5

Plot of $P_{fit}(r) - P_{num}(r)$ for 2s Orbital

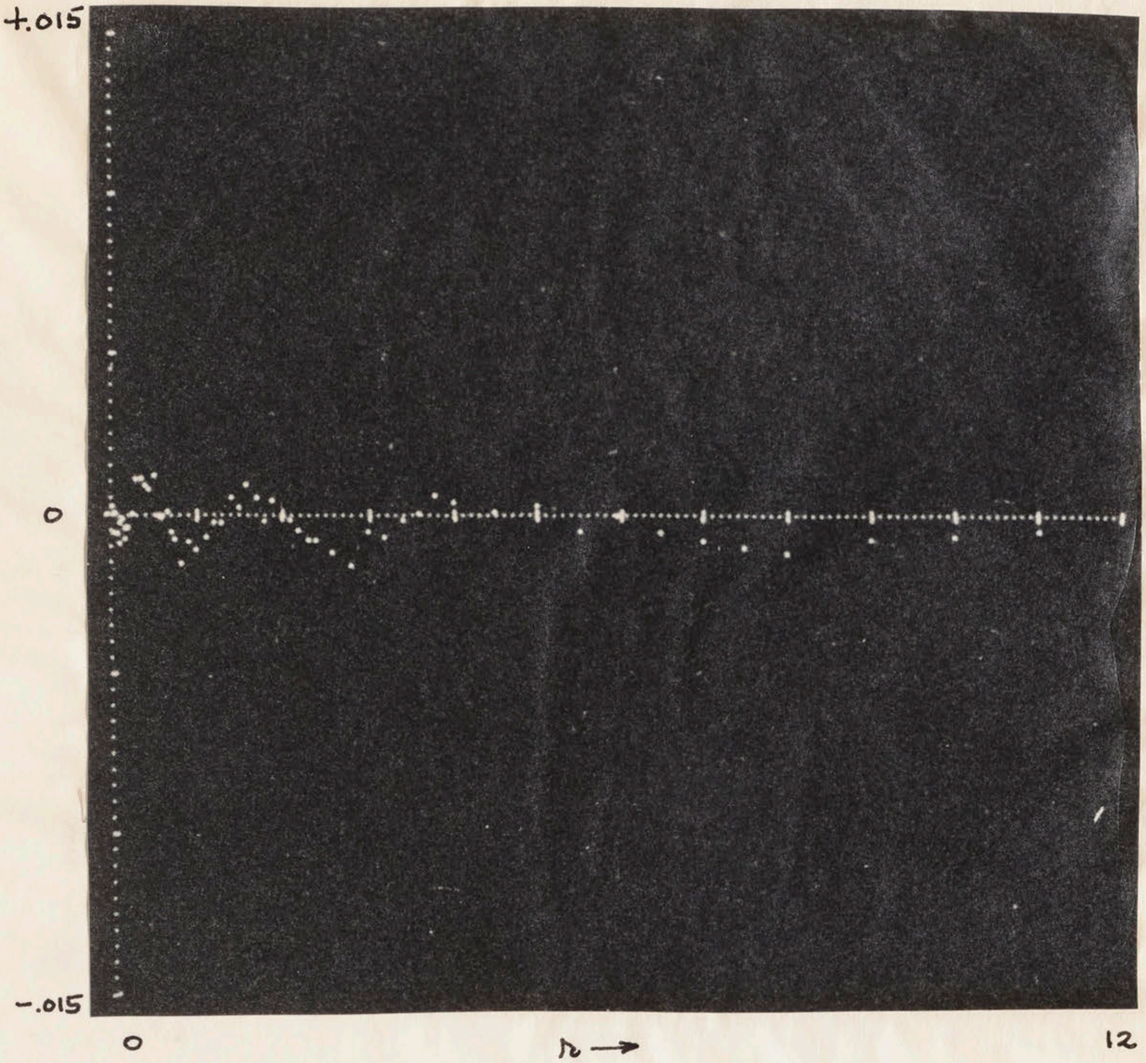


Fig. 3-6

Plot of $P_{fit}(r) - P_{num}(r)$ for 2p Orbital

Table 3-1

Parameters of the Analytic Fits to the ^3P Carbon Atomic Orbitals

The φ's designate normalized Slater AO's. The c_i's were determined by analytic renormalization.

1s orbital:

$$\psi_{1s}(\vec{r}) = (4\pi)^{-1/2} \sum_{i=1}^{3} a_i e^{-b_i r}$$

$$= \sum_{i=1}^{3} c_i \varphi(1s|b_i|\vec{r})$$

i	a_i	b_i	c_i
1	3.967302	9.518314	.06755376
2	23.51620	5.459509	.9217881
3	.2187563	3.122886	.01982078

2s orbital:

$$\psi_{2s}(\vec{r}) = (4\pi)^{-1/2}(0.3750000 - r) \sum_{i=1}^{3} a_i e^{-b_i r}$$

$$= \sum_{i=1}^{3} c_i' \varphi(1s|b_i|\vec{r}) + \sum_{i=1}^{3} c_i'' \varphi(2s|b_i|\vec{r})$$

i	a_i	b_i	c_i'	c_i''
1	4.682416	5.465749	+.06871681	−.05806877
2	8.667200	2.579525	+.3923166	−.7024676
3	2.356427	1.428921	+.2587076	−.8362388

2p orbital:

$$\psi_{2pz}(\vec{r}) = \left(\frac{3}{4\pi}\right)^{1/2} P_1(\cos\theta) \sum_{i=1}^{3} a_i e^{-b_i r}$$

$$= \sum_{i=1}^{3} c_i \varphi(2pz|b_i|\vec{r})$$

i	a_i	b_i	c_i
1	2.061680	4.459757	.04253098
2	2.943143	2.013452	.4433229
3	.8774781	1.110318	.5853019

The potential function, $Z_p(r)$ which was also fitted, is given in fig. 3-7. Careful inspection of the function on a semi-log graph revealed a negative second derivative in one region so that in order to fit accurately, at least one of the exponentials used for fitting had to have a negative coefficient. Consequently, a slight modification of the previous orbital fitting scheme was required; namely, it was necessary to start the iterative process as though several iterations had already occured. This required a guess for the initial a_i and b_i ; it was found that a 4-exponential fit gave satisfactory accuracy. The resultant error function is plotted in fig. 3-8. Table 3-2 gives the parameters of the fit, and Table 3-3 gives the generated numerical values of the fitted Z_p function.

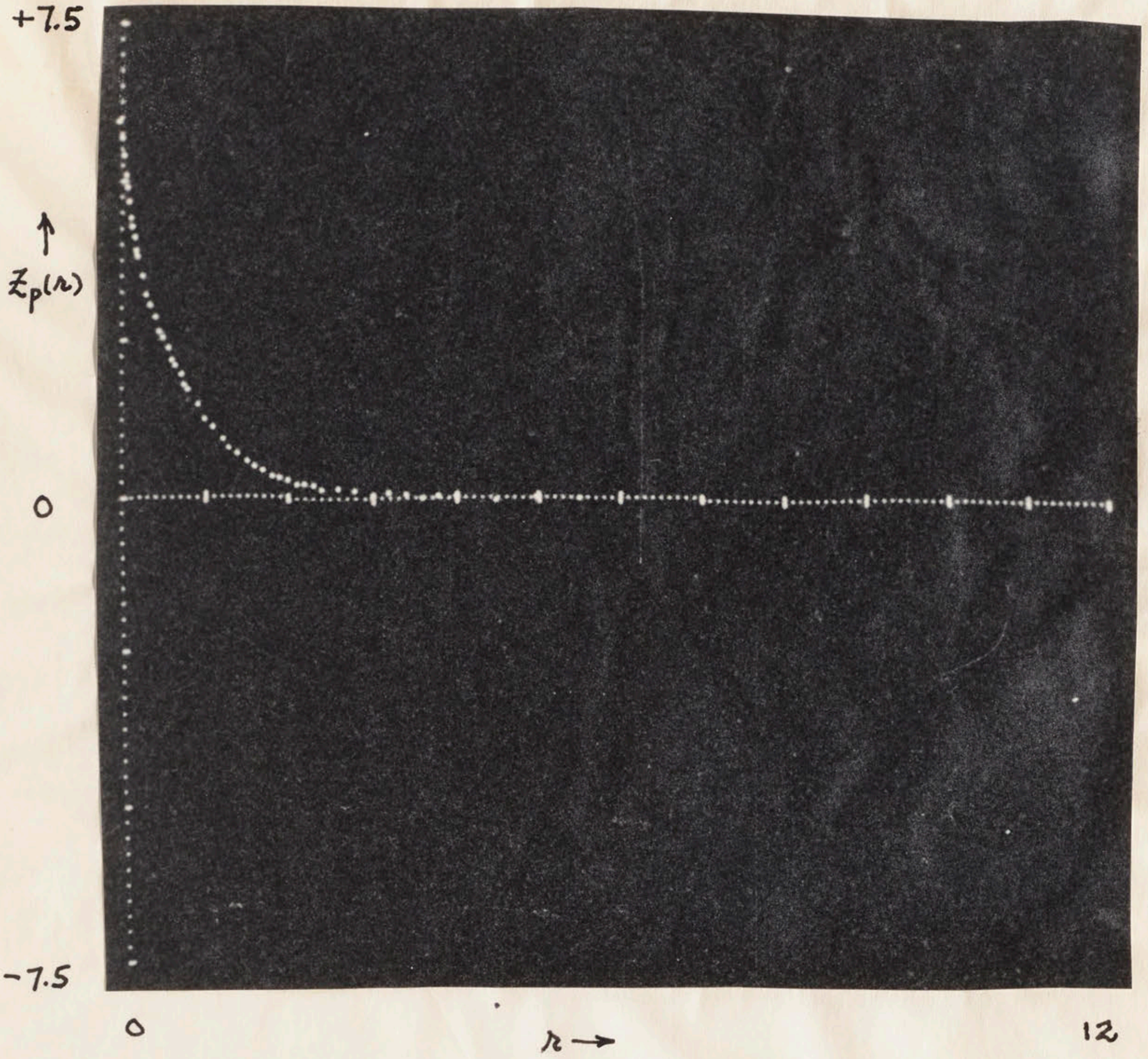


Fig. 3-7
Plot of $Z_p(r)$

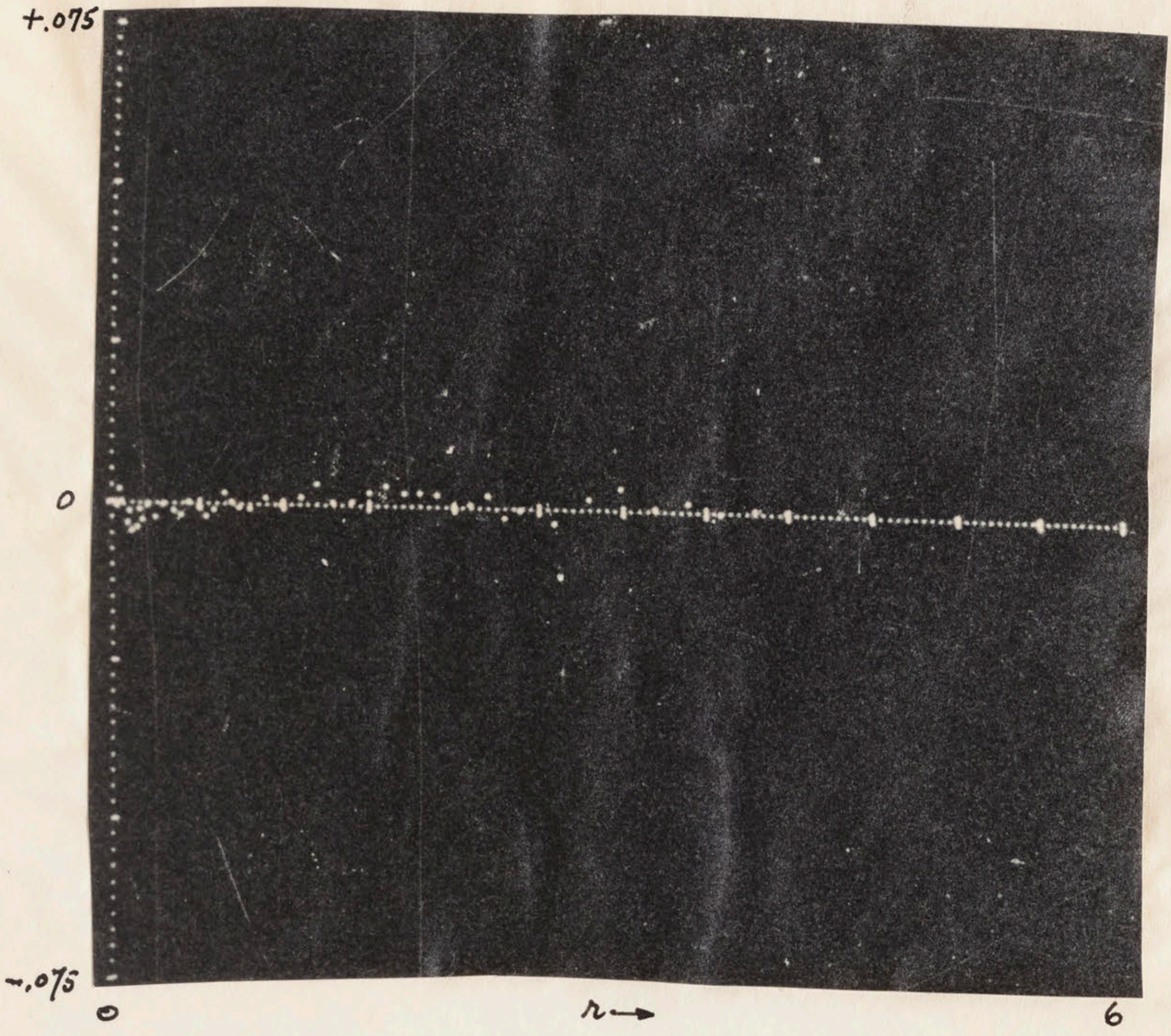


Fig. 3-8

Plot of $Z_{p\ fit}(r) - Z_{p\ num}(r)$

Table 3-2

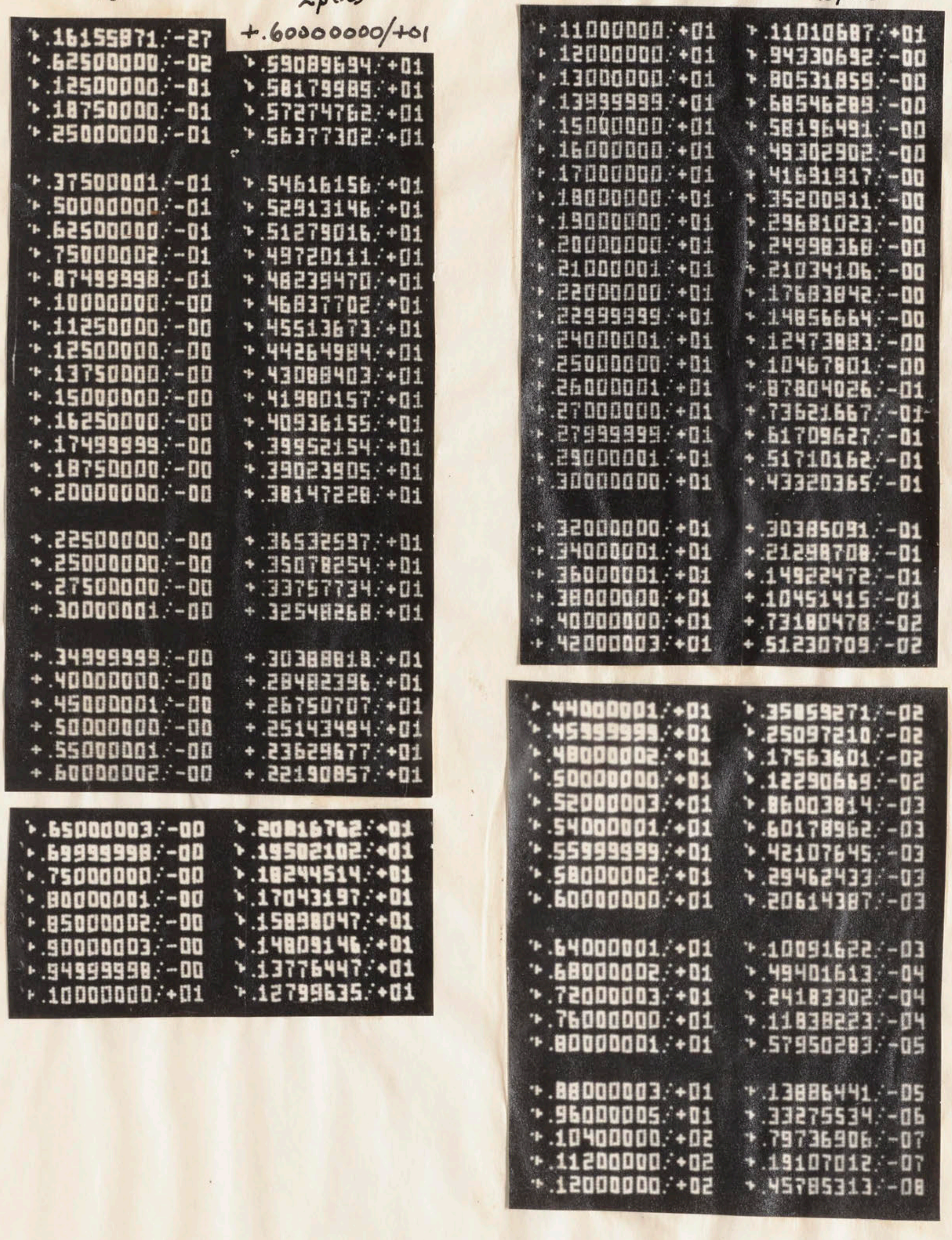
Parameters of the Analytic Fit to the Z_p Function

$$Z_p(r) = \sum_{i=1}^{4} a_i e^{-b_i r}$$

i	a_i	b_i
1	- 1.079855	18.46454
2	+ 8.842369	7.047181
3	-14.32999	3.240927
4	+18.56748	1.785846

Table 3-3

Numerical values of the analytic fit to $Z_p(r)$ given on the mesh used for the numerical quadratures described in chapter 5.



r	$Z_p(r)$
+.16155871.-27	+.60000000/+01
+.62500000.-02	+.59089694.+01
+.12500000.-01	+.58179989.+01
+.18750000.-01	+.57274762.+01
+.25000000.-01	+.56377302.+01
+.37500001.-01	+.54616156.+01
+.50000000.-01	+.52913146.+01
+.62500000.-01	+.51279016.+01
+.75000002.-01	+.49720111.+01
+.87499998.-01	+.48239470.+01
+.10000000.-00	+.46837702.+01
+.11250000.-00	+.45513673.+01
+.12500000.-00	+.44264984.+01
+.13750000.-00	+.43088403.+01
+.15000000.-00	+.41980157.+01
+.16250000.-00	+.40936155.+01
+.17499999.-00	+.39952154.+01
+.18750000.-00	+.39023905.+01
+.20000000.-00	+.38147228.+01
+.22500000.-00	+.36532597.+01
+.25000000.-00	+.35078254.+01
+.27500000.-00	+.33757734.+01
+.30000001.-00	+.32548268.+01
+.34999999.-00	+.30388818.+01
+.40000000.-00	+.28482396.+01
+.45000001.-00	+.26750707.+01
+.50000000.-00	+.25143494.+01
+.55000001.-00	+.23629677.+01
+.60000002.-00	+.22190857.+01
+.65000003.-00	+.20816762.+01
+.69999998.-00	+.19502102.+01
+.75000000.-00	+.18244514.+01
+.80000001.-00	+.17043197.+01
+.85000002.-00	+.15898047.+01
+.90000003.-00	+.14809146.+01
+.94999998.-00	+.13776447.+01
+.10000000.+01	+.12799635.+01
+.11000000.+01	+.11010687.+01
+.12000000.+01	+.94330692.-00
+.13000000.+01	+.80531859.-00
+.13999999.+01	+.68546289.-00
+.15000000.+01	+.58196491.-00
+.16000000.+01	+.49302902.-00
+.17000000.+01	+.41691917.-00
+.18000000.+01	+.35200911.-00
+.19000000.+01	+.29681023.-00
+.20000000.+01	+.24998368.-00
+.21000001.+01	+.21034106.-00
+.22000000.+01	+.17683842.-00
+.22999999.+01	+.14856664.-00
+.24000001.+01	+.12473883.-00
+.25000000.+01	+.10467801.-00
+.26000001.+01	+.87804026.-01
+.27000000.+01	+.73621667.-01
+.27999999.+01	+.61709627.-01
+.29000001.+01	+.51710162.-01
+.30000000.+01	+.43320365.-01
+.32000000.+01	+.30385091.-01
+.34000001.+01	+.21298708.-01
+.36000001.+01	+.14922472.-01
+.38000000.+01	+.10451415.-01
+.40000000.+01	+.73180478.-02
+.42000003.+01	+.51230709.-02
+.44000001.+01	+.35859271.-02
+.45999999.+01	+.25097210.-02
+.48000002.+01	+.17563601.-02
+.50000000.+01	+.12290669.-02
+.52000003.+01	+.86003814.-03
+.54000001.+01	+.60178962.-03
+.55999999.+01	+.42107645.-03
+.58000002.+01	+.29462433.-03
+.60000000.+01	+.20614387.-03
+.64000001.+01	+.10091622.-03
+.68000002.+01	+.49401613.-04
+.72000003.+01	+.24183302.-04
+.76000000.+01	+.11838223.-04
+.80000001.+01	+.57950283.-05
+.88000003.+01	+.13886441.-05
+.96000005.+01	+.33275534.-06
+.10400000.+02	+.79736906.-07
+.11200000.+02	+.19107012.-07
+.12000000.+02	+.45785313.-08

The negative second derivative of the function $\ln Z_p$ (or equivalently of Z_p itself), requires further discussion. This is because the second derivative of Z_p must be positive definite as indicated by the equation

$$\frac{d^2 Z_p(r)}{dr^2} = \frac{P^2(r)}{r} \qquad (3\text{-}15)$$

where

$$P^2(r) = \sum{}' (2l+1) P_{nl}^2(r) \quad ,$$

the P_{nl}^2 are the radial probability functions of the orbitals, and the primed sum is taken over all the occupied orbitals. This inconsistency in the tabulated Z_p function was not realized until late in the calculation. Further investigation has shown that the negative second derivative represents simple numerical error in Freeman's Z_p function. In particular, the Z_p function was recomputed from the integral equation

$$Z_p(r) = Z - \left\{ \int_0^r P^2(r')dr' + r\int_r^\infty \frac{P^2(r')}{r'} dr' \right\} \qquad (3\text{-}16)$$

using the analytic fits of the atomic orbitals and the generation and integration machinery described in Chapter 5. The latter Z_p was compared with the analytic fit to Freeman's Z_p ; the magnitude of the maximum error was found to be .006, a value about equal to the original fitting error indicated in fig. 3-8. Thus it appears that Freeman's data had more numerical error in it than expected. It is clear though that this error did not affect the present calculation except in the sense of unnecessary fitting difficulties.

Chapter 4

Evaluation of Two-Center Integrals

This chapter is primarily concerned with the computation of the previously defined $S_{jj'}$ and $T_{jj'}$ integrals of Chapter 2. The reader therefore may conveniently skip this chapter if he so desires. The basic evaluation technique is that which has been developed for the computation of two-center integrals between analytic Slater AO's [13, 14] and consists of transforming the integrals into prolate spheroidal coordinates. When this is done, it is found that all two-center, one-electron integrals are expressible as linear combinations of the auxiliary functions $A_n(x)$ and $B_n(x)$. The later functions are readily computable by relatively standard procedures which are described in a recent article by the writer, given as Appendix A.

To illustrate briefly the technique, a two-center overlap integral between 1s Slater AO's is derived. The normalized 1s orbital is defined as

$$\varphi(100|\kappa|\vec{r}) = \frac{\kappa^{3/2}}{\pi^{1/2}} e^{-\kappa r} \tag{4-1}$$

so that the overlap integral between a 1s orbital on center 1 and a 1s orbital on center 2 at a distance a apart is

$$\langle 100|100\rangle = \int \varphi(100|\kappa_1|\vec{r}_1)\,\varphi(100|\kappa_2|\vec{r}_2)\,d\tau \tag{4-2}$$

Using prolate spheroidal coordinates ξ, η, φ where

$$r_1 = (\xi+\eta)\,a/2 \tag{4-3}$$

$$r_2 = (\xi-\eta)\,a/2$$

$$d\tau = \frac{a^3}{8}(\xi^2-\eta^2)\,d\xi\,d\eta\,d\varphi$$

one easily obtains

$$\langle 100|100\rangle = \frac{(K_1K_2)^{3/2}}{8\pi} a^3 \int_0^{2\pi} d\varphi \int_{-1}^{1} d\eta \int_1^{\infty} d\xi \, (\xi^2-\eta^2)\, e^{-\xi\rho} e^{-\eta\sigma} \tag{4-4}$$

where $\rho = (K_1+K_2)a/2$ and $\sigma = (K_1-K_2)a/2$

By definition of the auxiliary functions

$$C_n(\rho) = \rho^{n+1} e^{\rho} \int_1^{\infty} \xi^n e^{-\xi\rho} d\xi = \rho^{n+1} e^{\rho} A_n(\rho) \tag{4-5}$$

and

$$B_n(\sigma) = \int_{-1}^{1} \eta^n e^{-\eta\sigma} d\eta \tag{4-6}$$

one finds that

$$\langle 100|100\rangle = 2\, \frac{(K_1K_2)^{3/2}}{(K_1+K_2)^3}\, e^{-\rho} \left[B_0(\sigma) C_2(\rho) - \rho^2 B_2(\sigma) C_0(\rho) \right] \tag{4-7}$$

The choice of the C_n rather than the A_n function was because the C_n are not singular for $\rho=0$ and therefore the two-center integral is conveniently evaluated for any distance without the spurious introduction of singularities from the A_n functions.

The above technique works equally well on the higher quantum number Slater AO's without any particular complications. The kinetic energy integrals are also simple inasmuch as the function $\nabla^2\varphi(nlm)$ is a linear combination of $\varphi(nlm)$, $\varphi(n-1,lm)$ and $\varphi(n-2,lm)$. Finally the two-center potential integrals where a function $\frac{1}{r}e^{-Kr}$ is placed on center 1, one Slater AO on center 2, and the other Slater AO on center 1 or 2, are easily evaluated in the same way as the above overlap integral.

The A_n and B_n functions are tabulated sparsely by Kotani, et al,[15] but, inasmuch as the labor of interpolation would have been severe without even considering the human reliability problem, it was felt that a C_n and B_n subroutine for the Whirlwind computer would be desirable. Such a subroutine was written and tested against the Kotani tables; the subroutine used simple upward recursion to obtain the C_n and a reformulation in terms of spherical Bessel function of imaginary argument to compute the more difficult B_n functions. The basis of this subroutine is described in Appendix A.

With the C_n and B_n generation subroutine available, an integral combining program was then written. This program computed the overlap, kinetic energy and potential integrals between the carbon Hartree-Fock orbitals which had been fitted with Slater AO's and the similarly fitted potential function. Thus the orbital input data was of the form

$$\psi(\vec{r}) = \sum_i c_i \, \varphi(\kappa_i|\vec{r}) \qquad (4\text{-}8)$$

and the potential of the form

$$V(\vec{r}) = \frac{1}{r} \sum_i c_i \, e^{-\kappa_i r} \qquad (4\text{-}9)$$

where the φ are the analytic Slater AO's. It is pertinent to remark that the combining program required as much effort to create as the original C_n and B_n subroutine. Inasmuch as the Hartree-Fock orbitals in general required three Slater AO's for a fit, this meant that a single overlap or kinetic energy integral between Hartree-Fock orbitals required 9 basic integrals between Slater AO's. Similarly for the potential integrals, because of the four exponential fit of the potential, there were 36 basic integrals per resultant integral between

Hartree-Fock orbitals and potential. Each of these basic Slater AO integrals required from one to two seconds of machine time to compute and were obtainable with six to seven figure accuracy.

It should be clear from the preceding remarks, that these explicit two-center methods become less efficient for applications involving atomic orbitals expressed as linear combinations of Slater AO's, in contrast to the multi-center techniques given in the next chapter. In fact, as soon as the general two-electron integral is considered, the efficiency loss is profound. However, for the present calculation, the advantages of easy operation and known accuracy behavior more than offset any computer time which might have been saved. In addition, the comparisons possible between the two methods were important internal checks on the computations.

In summary, the foregoing method and combination procedures were used to compute all the two-center integrals, integrals which depend only upon the distance between the two centers. To be explicit, these integrals are the following, which were defined in Chapter 2.

$$S_{jj'}(\lambda\mu 0) = \int \psi_j^*(\vec{r}-\vec{\rho}_{\lambda\mu 0})\, \psi_{j'}(\vec{r}-\vec{\rho}_{000})\, d\tau \qquad (4\text{-}10)$$

$$T_{jj'}(\lambda\mu 0) = -\frac{1}{2}\int \psi_j^*(\vec{r}-\vec{\rho}_{\lambda\mu 0})\, \nabla^2 \psi_{j'}(\vec{r}-\vec{\rho}_{000})\, d\tau \qquad (4\text{-}11)$$

$$P_{jj'}(\lambda\mu\nu/000) = \int \psi_j^*(\vec{r}-\vec{\rho}_{\lambda\mu 0})\, V(\vec{r}-\vec{\rho}_{000})\, \psi_{j'}(\vec{r}-\vec{\rho}_{000})\, d\tau \qquad (4\text{-}12)$$

$$P_{jj'}(000/\lambda'\mu'\nu') = \int \psi_j^*(\vec{r}-\vec{\rho}_{000})\, V(\vec{r}-\vec{\rho}_{\lambda'\mu'\nu'})\, \psi_{j'}(\vec{r}-\vec{\rho}_{000})\, d\tau \qquad (4\text{-}13)$$

where $j, j' = 1s, 2s, 2p\sigma, 2p\pi, 2p\bar{\pi}$ and $\sigma, \pi, \bar{\pi}$ refer to the two-center axis as described by fig. 2-4 of Chapter 2.

Chapter 5

Evaluation of Three-Center Integrals

In this chapter the evaluation of the previously defined $P_{jj'}(\lambda\mu o|\lambda'\mu'\nu')$ integrals will be described. To evaluate the three-center integrals, the procedure used is a very general one capable of being used on all multi-center integrals between atomic orbitals[16]. As might be expected, however, the computation rapidly becomes complex for the more general classes of integrals. The procedure consists of taking all atomic wave functions, described in spherical coordinates around one center in space and expanding in spherical coordinates about another center, in particular, the center of the atomic potential function, $V(\vec{r})$; in this application; then the resultant single-center integrals are calculated by numerical quadrature. Much of this procedure is not new, having been examined previously by Coolidge[17], Barnett and Coulson[18], Lowdin[19] and others, but there are many detailed conventions which must be consistently adhered to. Inasmuch as the exact methods used do not follow any of the aforementioned writers' conventions, but instead were developed independently, they will be given now.

In particular, the expansion of a normalized complex Slater AO is defined, the consideration of real Slater AO's being treated later. The definition is:

$$\varphi(nlm|\kappa|\vec{r}) = M(nlm|\kappa)\,\kappa\,(\kappa r)^{n-1} e^{-\kappa r} P_l^{|m|}(\cos\theta)\,\Phi_m(\varphi) \qquad (5\text{-}1)$$

where $$M(nlm|\kappa) = \left[\frac{2^{2n}\,\kappa\,(2l+1)}{(2n)!}\frac{(l-|m|)!}{(l+|m|)!}\right]^{1/2}$$

$$\Phi_m(\varphi) = (2\pi)^{-1/2} e^{im\varphi}$$

For convenience the unnormalized Slater AO is also defined

$$v(n\ell m|\kappa|\vec{r}) = \left[M(n\ell m|\kappa)\right]^{-1}\varphi(n\ell m|\kappa|\vec{r}) \qquad (5\text{-}2)$$

Then in terms of the coordinates of fig. 5-1, the expansions about the center $r=0$ can be written

$$\varphi(n\ell m|\kappa|\vec{r}\,') = \sum_{j=|m|}^{\infty}(2j+1)\,\frac{\alpha_j(n\ell m|\kappa|a|r)}{r}\,P_j^{|m|}(\cos\theta)\,\Phi_m(\varphi) \qquad (5\text{-}3)$$

$$v(n\ell m|\kappa|\vec{r}\,') = \sum_{j=|m|}^{\infty}(2j+1)\,\frac{\beta_j(n\ell m|\kappa a|\kappa r)}{r}\,P_j^{|m|}(\cos\theta)\,\Phi_m(\varphi) \qquad (5\text{-}4)$$

so that

$$\alpha_j(n\ell m|\kappa|a|r) = M(n\ell m|\kappa)\,\beta_j(n\ell m|\kappa a|\kappa r) \qquad (5\text{-}5)$$

The choice of the form of the α_j functions was suggested by the resultant simplicity in the final integral formulas. The absolute value signs on m serve to make the α_j functions depend only on $|m|$, thereby reducing the functions required and also eliminating the usual confusion over the conventions for spherical harmonics of negative m. Further, the straightforward result

$$\beta_j(\nabla^2 n\ell m|\kappa a|\kappa r) = \kappa^2\left[\beta_j(n\ell m|\kappa a|\kappa r) - 2n\,\beta_j(n-1,\ell m|\kappa a|\kappa r) + (n+\ell)(n-\ell-1)\,\beta_j(n-2,\ell m|\kappa a|\kappa r)\right] \qquad (5\text{-}6)$$

is given where the notation $\beta_j(\nabla^2 n\ell m|\kappa a|\kappa r)$ means the expansion function corresponding to the function $\nabla^2 v(n\ell m|\kappa|\vec{r}\,')$ Thus it is clear that the expansion problem depends entirely on the β_j functions. In addition, the expansion functions of Hartree-Fock AO's which have been fitted by a linear combination of Slater AO's can be obtained by the same linear combination of the corresponding α_j functions of the Slater AO's.

The computation of the β_j functions is next considered. By rewriting an expression given by Watson[20] in terms of spherical Bessel functions of imaginary argument, one finds after using the coordinates described by fig 5-1 that

$$\frac{e^{-\kappa r'}}{\kappa r'} = \sum_{j=0}^{\infty} (2j+1)\, i_j\, k_j\, P_j(\cos\theta) \qquad (5\text{-}7)$$

where $i_j = i_j(\sigma)$, $k_j = k_j(\rho)$, σ and ρ being the lesser and greater, respectively of $\kappa a, \kappa r$. By differentiating with respect to κ one obtains the numerically accurate form,

$$e^{-\kappa r'} = \sum_{j=0}^{\infty} (2j+1) \left[\rho\, i_j\, k_{j-1} - \sigma\, i_{j+1}\, k_j \right] P_j(\cos\theta) \qquad (5\text{-}8)$$

To abbreviate the notation in the following discussion, the variables κa and κr are dropped from the β_j functions. Then from the two preceding relations and the definition of the $\beta_j(nlm)$ functions, one immediately obtains

$$\beta_j(000) = \kappa r\; i_j\, k_j \qquad (5\text{-}9)$$

$$\beta_j(100) = \kappa r \left[\rho\, i_j\, k_{j-1} - \sigma\, i_{j+1}\, k_j \right] \qquad (5\text{-}10)$$

which clearly depend on only the spherical Bessel functions of imaginary argument.

The i_j functions are the same functions as those used to generate the B_n auxiliary functions discussed in the preceding chapter. The generation of the i_j and B_n functions is described in a recently published paper by the writer, given in Appendix A. A more extensive discussion of the generation of both the i_j and k_j can be found in a recent progress report[21]

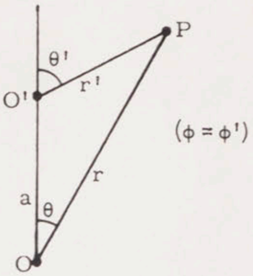
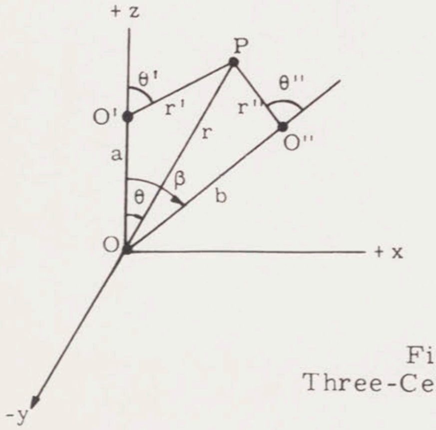


Fig. 5-1
Relation of Coordinates



φ = 0 half-plane includes + x axis and O''
φ' = 0 half-plane includes + x axis and O''
φ'' = π half-plane includes + z axis

Fig. 5-2
Three-Center Geometry

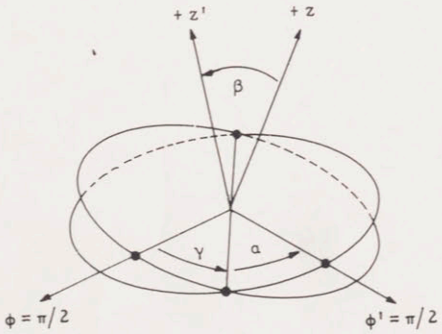


Fig. 5-3
Eulerian Angles

of the Solid-State and Molecular Theory Group with which the writer has been associated. A comprehensive description of the generation procedures for spherical Bessel functions of both real and imaginary arguments is the subject of a paper which is being prepared for publication with co-author J. Uretsky.

Returning to the β_j functions, one could laboriously build up higher quantum numbers by continued differentiation of eqs. 5-7 and 5-8. Instead a recursion scheme turns out to be much simpler to apply. From fig. 5-1 the following geometric relations are observed.

$$(r')^2 = a^2 + r^2 - 2ar\cos\theta \qquad (5\text{-}11)$$

$$r'\cos\theta' = -a + r\cos\theta \qquad (5\text{-}12)$$

$$r'\sin\theta' = r\sin\theta \qquad (5\text{-}13)$$

By multiplying the defining equation 5-4 for the β_j function by each of eqs. 5-11, 5-12, and 5-13 and then using the recursion formulas for Legendre polynomials

$$(2n+1)\cos\theta\, P_n^{|m|}(\cos\theta) = (n-|m|+1)P_{n+1}^{|m|}(\cos\theta) + (n+|m|)P_{n-1}^{|m|}(\cos\theta) \qquad (5\text{-}14)$$

$$(2n+1)\sin\theta\, P_n^{|m|}(\cos\theta) = P_{n+1}^{|m|+1}(\cos\theta) - P_{n-1}^{|m|+1}(\cos\theta) \qquad (5\text{-}15)$$

to reduce to a single summation, one obtains a set of recursion relations for the $\beta_j(nlm)$. To describe these relations succinctly, auxiliary operators are introduced.

If

$$U_j\,\beta_j(nlm) = \beta_{j+1}(nlm) \qquad (5\text{-}16)$$

$$L_j\,\beta_j(nlm) = \beta_{j-1}(nlm) \qquad (5\text{-}17)$$

and

$$\mathrm{X}_j = \frac{\kappa r}{2j+1}\left[L_j - U_j\right] \qquad (5\text{-}18)$$

$$Z_j = -\kappa a + \left(\frac{\kappa r}{2j+1}\right)\Big[(j-|m|)L_j + (j+|m|+1)U_j\Big] \tag{5-19}$$

$$R_j^2 = (\kappa a)^2 + (\kappa r)^2 - \frac{2(\kappa a)(\kappa r)}{2j+1}\Big[(j-|m|)L_j + (j+|m|+1)U_j\Big] \tag{5-20}$$

then one obtains the recursion relations

$$\beta_j(a+2, bc) = R_j^2\, \beta_j(abc) \tag{5-21}$$

$$\beta_j(a+1, b+1, b+1) = (2b+1)\, X_j\, \beta_j(abb) \tag{5-22}$$

$$\beta_j(a+1, b+1, c) = \left(\frac{2b+1}{b-|c|+1}\right) Z_j \beta_j(abc) - \left(\frac{b+|c|}{b-|c|+1}\right) R_j^2 \beta_j(a-1, b-1, c) \tag{5-23}$$

where in the last relation $\beta_j(a-1, b-1, b)$ is to be taken as zero.

The recursion scheme then proceeds as follows. Starting with the set $\beta_j(000)$ if $n-l$ is even or $\beta_j(100)$ if $n-l$ is odd, for all the required j values plus n extra, we recurse using eq. 5-21 until $\beta_j(n-l, 00)$ is reached. Eq. 5-22 is then applied m times to $\beta_j(n-l, 00)$ to yield $\beta_j(n-l+m, mm)$. The latter result along with the relation $\beta_j(n-l+m, m, m+1) = 0$ is used to start the upward recursion of eq. 5-23; after l-m steps, the desired set of $\beta_j(nlm)$ are obtained.

The numerical properties of the above recursion scheme are not completely known, although, inspection indicates no obvious problems. However, before this recursion scheme was fully worked out, a generation program was written for the Whirlwind computer which used the R_j^2, X_j and Z_j operators to construct the expansion functions of the atomic orbitals with quantum numbers nlm equal to: 000 100, 200, 300, 110, 210, 310, 111, 211, 311. No noticeable numerical failures have appeared with these expansion functions.

Having seen how the β_j functions and thus the α_j functions are generated, it is now possible to derive certain integral formulas. Considering first the 2-center overlap and kinetic energy integrals, and using the coordinates of fig. 5-1 , it then follows that

$$\langle n_1 l_1 m_1 | n_2 l_2 m_2 \rangle \equiv \int \varphi^*(n_1 l_1 m_1 | K_1 | \vec{r}) \, \varphi(n_2 l_2 m_2 | K_2 | \vec{r}\,') \, d\tau \tag{5-24}$$

$$= \int (2l_1+1) \, \alpha_{l_1}(n_1 l_1 m_1 | K_1 | 0 | r) \, P_{l_1}^{|m_1|}(\cos\theta) \, \Phi_{m_1}^*(\varphi) \cdot$$

$$\cdot \sum_{j=|m_2|}^{\infty} (2j+1) \, \alpha_j(n_2 l_2 m_2 | K_2 | a | r) \, P_j^{|m_2|}(\cos\theta) \, \Phi_{m_2}(\varphi) \, dr \, d(\cos\theta) \, d\varphi$$

Integrating over the angular funtions and using the orthonormality relations

$$\int_0^{2\pi} \Phi_{m_1}^*(\varphi) \, \Phi_{m_2}(\varphi) \, d\varphi = \delta(m_1, m_2) \tag{5-25}$$

$$\int_{-1}^{1} P_{l_1}^{|m|}(\mu) \, P_{l_2}^{|m|}(\mu) \, d\mu = \delta(l_1, l_2) \, \frac{2}{2l_1+1} \, \frac{(l_1+|m|)!}{(l_1-|m|)!} \tag{5-26}$$

one obtains

$$\langle n_1 l_1 m_1 / n_2 l_2 m_2 \rangle = \delta(m_1, m_2) \, 2 \, (2l_1+1) \frac{(l_1+|m_1|)!}{(l_1-|m_1|)!} \int_0^{\infty} \alpha_{l_1}(n_1 l_1 m_1 | K_1 | 0 | r) \, \alpha_{l_1}(n_2 l_2 m_2 | K_2 | a | r) \, dr \, . \tag{5-27}$$

The last formula holds also for $n_1 l_1 m_1$ replaced by $\nabla^2 n_1 l_1 m_1$ Thus the overlap and kinetic energy integrals can be done by a single numerical quadrature of a rather-difficult-to-obtain integrand. It was for the latter reason that the overlap and kinetic energy integrals used in the present calculation were those obtained by the use of the more convenient and precise 2-center integral techniques described in the previous chapter.

However, values were spot-checked by means of the numerical quadrature method given here and were found to be in agreement with the 4 to 6 decimal figure accuracy of the numerical quadratures.

Formally eq. 5-27 also holds for $n_2 l_2 m_2$ replaced by $\nabla^2 n_2 l_2 m_2$ but practically is a very poor form to use. The reason for this is that the expansion functions of $\nabla^2 \varphi(nlm)$ are much more localized as a function of the variable r than are the corresponding expansion functions of $\varphi(nlm)$. In fact, the expansion functions of $\nabla^2 \varphi(100)$ actually have a cusp-like behavior (i.e. discontinuous first-derivative) at $r = a$. Consequently a numerical quadrature, which is based on a finite number of integrand points and assumed continuity of integrand derivatives, must be done with particular care if accuracy is to be maintained.

In order to treat the 3-center potential integrals involving two atomic wave functions and an atomic potential by the presently discussed methods, it is clear that two of the three functions must be expanded about another center. With reference to fig. 5-2 it would be simplest to place one wave function on center O, another on center O$'$, the potential function on center O", and then expand all the functions about center O. Before the angular integrations can be performed, however, it is necessary to transform the spherical harmonics arising from the potential expansion along the OO" axis to the spherical coordinates of the OO' axis. The usual addition theorem of spherical harmonics will accomplish this for a potential which is symmetric about the OO" axis. A serious drawback though will arise from the fact that the singular nature of the potential requires that the expansion functions have cusps at r = b. Thus the same difficulties in the numerical quadrature which arose with certain kinetic energy integrals will also occur here. A further difficulty arises from the fact that in order to generate the expansion functions of the potential by the techniques which have been described, it would be required to have the potential fitted by a linear combination of Slater AO's. Hence, in general, an arbitrary numerically-given potential could not be used, although in the present work a fitted potential was used.

The difficulties which arise from expanding the potential function are obviously avoided if instead both wave functions are expanded about the center of the potential. However, a new complication arises in that the usual spherical harmonic addition theorem will no longer suffice in general to transform the spherical harmonics from the coordinates of one expansion axis to those of the other. Therefore the general rotation of spherical harmonics will next be discussed.

The coefficients describing the rotation of spherical harmonics are defined as

$$P_\ell^{|m'|}(\cos\theta')\,\Phi_{m'}(\varphi') = \sum_{m=-\ell}^{\ell} \frac{(\ell-|m|)!}{(\ell+|m|)!}\, F_\ell^{m'm}(\beta)\, e^{-im'\alpha} e^{-im\gamma} P_\ell^{|m|}(\cos\theta)\,\Phi_m(\varphi) \qquad (5\text{-}28)$$

where α, β, γ are in this equation the Eulerian angles of rotation of the unprimed to the primed coordinate axes. To be unambiguous the exact prescription for rotating the axes is given where all rotations are in a right-hand screw sense.

1. Rotate the $\varphi = \pi/2$ line in the x-y plane about the $+z$ axis until it intercepts the x' - y' plane. Call this angle γ .
2. Rotate the $+z$ axis about the new $\varphi = \pi/2$ axis in the x' - y' plane until it coincides with the $+z'$ axis. Call this angle β .
3. Rotate the new $\varphi = \pi/2$ axis in the x' - y' plane about the $+z'$ axis until it coincides with the $\varphi' = \pi/2$ axis in the x' - y' plane. Call this angle α .

Fig. 5-3 illustrates these angles. The particular rotation formula given by eq. 5-28 has been chosen because for m'= 0, there results the ordinary addition theorem of spherical harmonics where $F_\ell^{0m}(\beta) = P_\ell^{|m|}(\cos\beta)$.

The formula for the F functions can be deduced from a formula of Wigner[22]. Wigner ambiguously states his normalization and his Eulerian angles, besides using a left-handed coordinate system. After elimination of all these confusing factors, the following formula was obtained.

$$F_\ell^{m'm}(\beta) = (-1)^{\frac{1}{2}(m+|m|+m'+|m'|)} (\ell+|m|)!\,(\ell+|m'|)! \sum_t (-1)^t \frac{(\cos\beta/2)^{2\ell+m'-m-2t}\,(\sin\beta/2)^{2t+m-m'}}{(\ell-m-t)!\,(\ell+m'-t)!\,(t+m-m')!\,t!} \qquad (5\text{-}29)$$

where t takes on all values giving non-negative factorials. The F function can also be expressed in terms of the hypergeometric function[23] which in turn is closely related to the Jacobi polynomial. For the case of $m \geq m'$

$$F_\ell^{m'm}(\beta) = (-1)^{\frac{1}{2}(m+|m|+m'+|m'|)} \frac{(\ell+|m|)!\,(\ell+|m'|)!}{(\ell-m)!\,(\ell+m')!} \frac{(\cos\beta/2)^{m+m'}(\sin\beta/2)^{m-m'}}{(m-m')!} F\left(m-\ell, \ell+m+1 \,\middle|\, m-m'+1 \,\middle|\, (\sin\beta/2)^2\right) \qquad (5\text{-}30)$$

By studying eqs. 5-28, 5-29 and 5-30 the following relations can be found.

$$\bar{F}_{\ell}^{mm'}(\beta) = \bar{F}_{\ell}^{-m,-m'}(\beta) = (-1)^{m+m'}\bar{F}_{\ell}^{m'm}(\beta) = (-1)^{m+m'}\bar{F}_{\ell}^{mm'}(-\beta) = (-1)^{\ell+m+m'}\bar{F}_{\ell}^{m,-m'}(\pi-\beta) \tag{5-31}$$

Having established the preceding relationships, it is now possible to consider the 3-center potential integrals. The following definition is made

$$\langle n_1 l_1 m_1 | V | n_2 l_2 m_2 \rangle = \int \varphi^*(n_1 l_1 m_1 | K_1 | \vec{r}\,') \, V(\vec{r}) \, \varphi(n_2 l_2 m_2 | K_2 | \vec{r}\,'') \, d\tau \qquad (5\text{-}32)$$

where $V(\vec{r})$ is a numerically given spherically symmetric potential having roughly the behavior of $\frac{1}{r} e^{-\kappa r}$, and the coordinates are those of fig. 5-2. When the wave functions are expanded about the O center, it then follows that the rotation of the spherical harmonics not expressed in terms of θ, φ is given by eq. 5-28 where $\alpha = \gamma = 0$. This leads to the expression

$$\langle n_1 l_1 m_1 | V | n_2 l_2 m_2 \rangle = \int \sum_j (2j+1) \alpha_j (n_1 l_1 m_1 | K_1 | a | r) P_j^{|m_1|}(\cos\theta) \, \Phi_{m_1}^*(\varphi) \, V(r) \underset{\overset{\uparrow}{P_k^{|m|}(\cos\theta)}}{\cdot} \qquad (5\text{-}33)$$

$$\cdot \sum_k (2k+1) \alpha_k (n_2 l_2 m_2 | K_2 | b | r) \sum_m \frac{(k-|m|)!}{(k+|m|)!} F_k^{m_2 m}(\beta) \, \Phi_m(\varphi) \, dr \, d(\cos\theta) \, d\varphi$$

After the usual integration over angles, one obtains

$$\langle n_1 l_1 m_1 | V | n_2 l_2 m_2 \rangle = 2 \sum_{j=0}^{\infty} (2j+1) F_j^{m_2 m_1}(\beta) \langle j | V | j \rangle \qquad (5\text{-}34)$$

where

$$\langle j | V | j \rangle = \int_0^\infty \alpha_j (n_1 l_1 m_1 | K_1 | a | r) \, V(r) \, \alpha_j (n_2 l_2 m_2 | K_2 | b | r) \, dr$$

In the present calculation the atomic orbitals of interest are the 1s, 2s, and 2p of Carbon. These real orbitals can be readily expressed in terms of the above complex orbitals of quantum numbers nlm by the transformations

$$(1s) \equiv (10\sigma') = (100) \qquad (5\text{-}35)$$

$$(2s) \equiv (20\sigma') = (200)$$

$$(2p\sigma') \equiv (21\sigma') = (210)$$

$$(2p\pi') \equiv (21\pi') = \frac{1}{\sqrt{2}} \left[(211) + (21,-1) \right]$$

$$(2p\bar{\pi}') \equiv (21\bar{\pi}') = \frac{1}{i\sqrt{2}} \left[(211) - (21,-1) \right]$$

where the σ', π' and $\bar{\pi}'$ refer to the usual symmetry with respect to the translation axes of the real atomic orbitals from the expansion center $r = 0$. The σ' and π' orbitals are even and the $\bar{\pi}'$ orbitals are odd with respect to reflection in the plane OO'O" of fig. 5-2. (It is noted that for descriptive convenience the axes of fig. 5-2 are permuted with respect to the axes of fig. 2-2, however because all further descriptions are of the σ, π -type no confusion will arise.) In terms of the real orbitals, one then obtains for the non-zero three-center integrals,

$$\langle n_1 l_1 \sigma' | V | n_2 l_2 \sigma' \rangle = 2 \sum_{j=0}^{\infty} (2j+1) F_j^{00}(\beta) \langle j | V | j \rangle \tag{5-36}$$

$$\langle n_1 l_1 \pi' | V | n_2 l_2 \sigma' \rangle = 2\sqrt{2} \sum_{j=0}^{\infty} (2j+1) F_j^{01}(\beta) \langle j | V | j \rangle \tag{5-37}$$

$$\langle n_1 l_1 \pi' | V | n_2 l_2 \pi' \rangle = 2 \sum_{j=0}^{\infty} (2j+1) \left[F_j^{11}(\beta) + F_j^{1,-1}(\beta) \right] \langle j | V | j \rangle \tag{5-38}$$

$$\langle n_1 l_1 \bar{\pi}' | V | n_2 l_2 \bar{\pi}' \rangle = 2 \sum_{j=0}^{\infty} (2j+1) \left[F_j^{11}(\beta) - F_j^{1,-1}(\beta) \right] \langle j | V | j \rangle \tag{5-39}$$

where the $\langle j | V | j \rangle$ still are the same as in eq. 5-34.

Several of the above sums were computed manually out to $j = 9$ with the convergence varying from good to poor. During computation an important point appeared, namely, that the $\langle j | V | j \rangle$ are in general monotonically decreasing with an approximate behavior of Ah^j where A and h are empirical constants depending on the integral involved. (An exception to the monotonicity occurs when one or both of the orbitals is a noded 2s function which has been fitted by a linear combination of 1s and 2s Slater AO's; however, the monotonicity is restored when the integrals involving 1s and 2s Slater AO components are evaluated separately.) For the cases of poor convergence, which correspond to the expansion of highly localized orbitals or large expansion distances, a correction procedure has been developed which will now be described.

Eqs. 5-36 to 5-39 are summarized in the form

$$\langle n_1 l_1 m_1 | V | n_2 l_2 m_2 \rangle = \sum_{j=0}^{\infty} G_j(\beta) \langle j | V | j \rangle \tag{5-40}$$

and can be rewritten as

$$\langle n_1 l_1 m_1 | V | n_2 l_2 m_2 \rangle = A\,H(\beta) + \sum_{j=0}^{N} G_j(\beta)\left[\langle j|V|j\rangle - Ah^j\right] + \sum_{j=N+1}^{\infty} G_j(\beta)\left[\langle j|V|j\rangle - Ah^j\right] \tag{5-41}$$

where

$$H(\beta) = \sum_{j=0}^{\infty} h^j G_j(\beta)$$

The correction procedure used is to adjust A and h so that the last sum from N + 1 to ∞ is approximately zero and can be neglected; simple fitting from $\langle N|V|N\rangle$ and $\langle N-1|V|N-1\rangle$ was found to be adequate. Before this procedure could be made useful however it was necessary to express the H functions in closed analytic form.

It can be shown by tedious identification through the hypergeometric function relation of the $F_j^{m_2 m_1}(\beta)$ functions that

$$F_j^{00}(\beta) = T_j^{0}(\beta) \tag{5-42}$$

$$F_j^{01}(\beta) = \sin\beta\, T_{j-1}^{1}(\beta) \tag{5-43}$$

$$\left[F_j^{11}(\beta) + F_j^{1,-1}(\beta)\right] = \frac{2}{2j+1}\left[j^2\, T_j^{1}(\beta) - (j+1)^2\, T_{j-2}^{1}(\beta)\right] \tag{5-44}$$

$$\left[F_j^{11}(\beta) - F_j^{1,-1}(\beta)\right] = 2\,T_{j-1}^{1}(\beta) \tag{5-45}$$

where the $T_n^m(\beta)$ are Gegenbauer polynomials^{24}. The generating function of the Gegenbauer polynomials is

$$\frac{(2m-1)!!}{D^{m+1/2}} = \sum_{j=0}^{\infty} h^j T_j^m(\beta) \tag{5-46}$$

where $D = 1 - 2h\cos\beta + h^2$

and $(2m-1)!! = (2m-1)(2m-3)(2m-5)\cdots 1$

After appropriate differentiation by h and β, formation of linear combinations and considerable involved algebra, there result the expressions

$$\sum_{j=0}^{\infty} (2j+1) h^j F_j^{00}(\beta) = \frac{1-h^2}{D^{3/2}} \tag{5-47}$$

$$\sum_{j=0}^{\infty} (2j+1) h^j F_j^{01}(\beta) = \frac{3h(1-h^2)\sin\beta}{D^{5/2}} \tag{5-48}$$

$$\sum_{j=0}^{\infty} (2j+1) h^j \left[F_j^{11}(\beta) + F_j^{1,-1}(\beta)\right] = \frac{6h(1-h^2)}{D^{5/2}} \left[\cos\beta - \frac{5h\sin^2\beta}{D}\right] \tag{5-49}$$

$$\sum_{j=0}^{\infty} (2j+1) h^j \left[F_j^{11}(\beta) - F_j^{-1,-1}(\beta)\right] = \frac{6h(1-h^2)}{D^{5/2}} \tag{5-50}$$

These results were checked by the alternative procedure of examining the $F_j^{m_2 m_1}(\beta)$ in terms of Jacobi polynomials and using the corresponding generating function; however, the complicated algebra did not particularly simplify.

The above tail-summation correction procedure was successful in giving the right order of magnitude for poorly convergent potential integrals, integrals whose values invariably turned out to be comparable to the numerical quadrature and summation truncation errors in the more important potential integrals. Thus it appears to be a good assumption that in more general calculations the elaborate tail-summation procedures are not necessary, provided the major integrals are obtained with sufficient accuracy. In any case, in the present calculation the tail-summation procedure served to ensure the accuracy of the potential integrals.

Having discussed the basic procedures for obtaining the three- center potential integrals, it remains to make the connection with the required $P_{jj'}(\lambda\mu 0|\lambda'\mu'\nu')$ which were defined and discussed in Chapter 2. From the definition

$$P_{jj'}(\lambda\mu 0|\lambda'\mu'\nu') = \int \psi_j^*(\vec{r}-\vec{\rho}_{\lambda\mu 0})\, V(\vec{r}-\vec{\rho}_{\lambda'\mu'\nu'})\, \psi_{j'}(\vec{r}-\vec{\rho}_{000})\, d\tau \tag{5-51}$$

where

$$j, j' = 1s, 2s, 2p\sigma, 2p\pi, 2p\bar{\pi}$$

and from fig. 5-2, it is clear that the center O must correspond to $\vec{\rho}_{\lambda'\mu'\nu'} = 0$, the center O' to $\vec{\rho}_{000} = 0$, and the center O" to $\vec{\rho}_{\lambda\mu 0} = 0$. However the ψ_j are not the atomic wave functions described by eq. 5-35 since they are angularly quantized with respect to the axis O'O" rather than to the axes OO' and OO". When j and j' are equal to the 1s, 2s, or $2p\bar{\pi}$ functions, which are invariant under rotation about an axis perpendicular to the plane OO'O", there is no difference between the two angular quantizations. However for the j or j' equal to $2p\sigma$ or $2p\pi$, there is an additional transformation required. The transformations are

$$\psi_{2p\sigma}(\vec{r}-\vec{\rho}_{000}) = \cos\gamma'\, \psi_{2p\sigma'}(\vec{r}-\vec{\rho}_{000}) + \sin\gamma'\, \psi_{2p\pi'}(\vec{r}-\vec{\rho}_{000}) \tag{5-52}$$

$$\psi_{2p\pi}(\vec{r}-\vec{\rho}_{000}) = -\sin\gamma'\, \psi_{2p\sigma'}(\vec{r}-\vec{\rho}_{000}) + \cos\gamma'\, \psi_{2p\pi'}(\vec{r}-\vec{\rho}_{000}) \tag{5-53}$$

and

$$\psi_{2p\sigma}(\vec{r}-\vec{\rho}_{\lambda\mu 0}) = \cos\gamma''\, \psi_{2p\sigma'}(\vec{r}-\vec{\rho}_{\lambda\mu 0}) - \sin\gamma''\, \psi_{2p\pi'}(\vec{r}-\vec{\rho}_{\lambda\mu 0}) \tag{5-54}$$

$$\psi_{2p\pi}(\vec{r}-\vec{\rho}_{\lambda\mu 0}) = \sin\gamma''\, \psi_{2p\sigma'}(\vec{r}-\vec{\rho}_{\lambda\mu 0}) + \cos\gamma''\, \psi_{2p\pi'}(\vec{r}-\vec{\rho}_{\lambda\mu 0}) \tag{5-55}$$

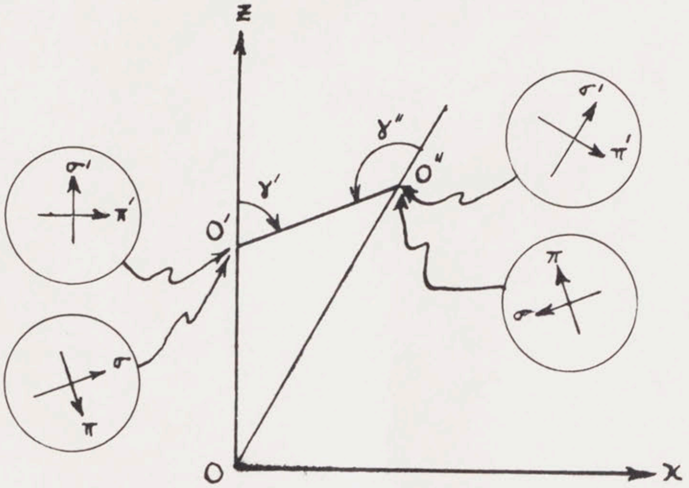


Fig. 5-4

Diagram of the x-z plane of fig. 5-2 showing the requantization of the $2p\sigma'$ and $2p\pi'$ orbitals into the $2p\sigma$ and $2p\pi$ orbitals.

where the angles are illustrated in fig. 5-4. Thus the integrals are in general a linear combination of four basic integrals when j and j' are 2p atomic orbitals. If higher symmetries of atomic orbitals had been used in this calculation, the above direct approach by inspection would have become much more difficult; the solution to this problem has already been established though in the $F_{\ell}^{m_2 m_1}(\beta)$ functions discussed earlier which allow one to make rotations of all spherical harmonics.

Having displayed all the details of evaluating the integrals, a summary of the whole procedure will now be given with particular reference to the scope of the computations and to the mechanizations which were used to carry out the procedures. The first stage of calculation involved the computation of the expansion functions, α_j, for the carbon atomic orbitals 1s, 2s (consisting of two nodeless sections: the 1s and 2s), 2pσ', and 2pπ' which had been fitted with linear combinations of Slater AO's. This was done on the computer with an α_j generation program which started from the fitting parameters of a given atomic orbital and computed the combined Slater AO expansion functions for the orbital. For each of the five nodeless atomic orbitals expanded at a given distance there were ten expansion functions, (or nine for the 2pπ' function), corresponding to a maximum-j equal to 9, or a total of 49 functions. For convenience, the generated expansion functions were punched out on paper tape by the computer in such a fashion that the functions could be automatically read back into the computer without any transcription or proofreading requirements. This generation and punchout process was done for expansion distances equal to the first four graphite neighbor distances; in addition, for the trivial case of zero expansion distance, the single non-zero expansion function for each of the four carbon atomic orbitals was generated and punched out. Thus the results at this stage consisted of a total of 200 functions each represented by a mesh of 82 points, giving a total of 16,400 numerical values. The machine time required to produce these expansion functions was about two hours. To indicate the unwieldiness of this quantity of numerical data, it has been estimated that it would take about an hour of machine time to merely automatically display all the numbers, not to mention the 400 frames of microfilm which the display would require.

The second stage of the potential integral computation consisted of evaluating from the multitude of α_j functions and the potential function the $\langle j|V|j\rangle$ numerical quadratures of eq. 5-34. This was accomplished on the computer by a specially written numerical quadrature program which was designed for easy operation. The 82 point numerical quadratures were done by Simpson's rule. The reason for using such a low order integration rule was the fact that the functions for the orbitals used at worst had discontinuous third and higher derivatives at the expansion distance. Consequently no extra integration error was introduced by not making the expansion distance a mesh point since Simpson's rule only assumes continuity up to and including the second derivative. The results of the numerical quadratures were also punched out onto paper tape by the computer in a fashion such that they could be automatically read back into the computer. All told there were about 2500 non-zero integrals which had to be computed in a fairly intricate sequence. The total machine time was about three hours for this process. The resultant numerical quadratures were also automatically displayed via microfilm for inspection and checking.

The third and final stage of the $P_{jj'}$ computation consisted of forming the summations of the numerical quadratures modulated by the $F_j^{m_2 m_1}(\beta)$ functions as indicated by eq. 5-36 to 5-39. For this purpose a special summation program was written which used a subroutine written for the purpose of generating the F functions by straight-forward application of eq. 5-29. In addition, the tail-summation correction procedure was incorporated in the program. Further features installed in the program were the transformation of the $\psi_{2p\sigma}$ and $\psi_{2p\pi'}$ indicated by eq. 5-51 to 5-55 and the consolidation, (after summation), of the two nodeless components of the noded carbon 2s orbital.

This program after evaluating the $P_{jj'}$ values also performed the elementary summation required to give the ultimately desired

$$V_{jj'}(\lambda\mu o) = \sum_{\lambda'\mu'\nu'} P_{jj'}(\lambda\mu o/\lambda'\mu'\nu') \qquad (5\text{-}56)$$

The results of the summation program then consisted of the individual $P_{jj'}$ and the resultant $V_{jj'}$. As a check on the correction procedure, two sets of simultaneous results were actually obtained, corresponding to the computation with and without the tail-summation correction procedure. The results were automatically recorded on microfilm and the total computer time for this last stage was about one hour.

A final comment should be made on the degenerate two-center cases of the $P_{jj'}$, which are important terms in a tight-binding calculation. Because the atomic orbitals were only expanded for the first four neighbors, the sum of $P_{jj'}$ involved in $V_{jj'}(000)$ were prematurely truncated; however because of the two-center degeneracy, and the fact that the potential function was analytically fitted, it was possible to compute, by the techniques of Chapter 4, the remaining terms and thus obtain the correct $V_{jj'}(000)$ values. These corrections were rather slight. Similarly in the general $V_{jj'}(\lambda\mu 0)$ summation, the important two-center terms were necessarily omitted in the numerical quadrature process for λ greater than four. These missing terms also were obtained by the two-center integral procedures of the previous chapter and used to correct the $V_{jj'}(\lambda\mu 0)$ values for λ greater than four.

Chapter 6

Application of the Whirlwind Computer

It is perhaps illuminating to give some of the computational perspective involved in the over-all calculation. Inasmuch as the magnitude of numerical work involved was such that accuracy would have been difficult to maintain in any hand calculation, most of the computational work was done on the high-speed electronic computer Whirlwind I. The nearly total mechanization of the problem, although eliminating almost entirely any possible random mistakes, had the disadvantage of tending to obscure possible systematic mistakes. The later shift of emphasis is one of the principal reasons that make the programming of a computer a non-trivial affair. A consequence is that logical simplicity of the computational procedure becomes a goal which is often in opposition to computational efficiency. There is also a great deal of difficulty in devising adequate test procedures for computer programs, since of necessity they must be tailored to the program itself. The ability of a programmer to cope with these problems develops mostly with experience. A large fraction of the time spent on the present calculation was thus used learning how to obtain the full potentiality of a high-speed computer.

In carrying out the calculation, the work fell into stages for each of which special computer programs were written. These were: a program for the semi-automatic fitting of the atomic orbitals and the Z_p function ; a program for generating the two-center integral auxiliary functions and then automatically combining terms to give the integrals between Hartree-Fock orbitals; a program for generating the atomic orbital expansion functions necessary for the three-center potential integrals; a program for performing the basic numerical quadratures of the three center potential integrals; and a requantization and summation program for forming the appropriate three-center integrals from the basic numerical quadratures. The foregoing computer programs were sufficient machinery to prepare the basic two-center Hamiltonian and overlap integrals which served as input for the final master program which performed the energy band calculation.

The computational steps covered by the above programs have been indicated in the block diagram given in fig. 6-1. Each solid-lined box of the diagram indicates a separate computational program which on the average took a few months to organize, write, trouble-shoot and test. In the case of the final master program, several programs of similar complexity were arranged to work automatically together as a single large program as indicated by the dotted enclosure.

The operation of the preparation programs have been described in Chapters 3, 4 and 5. These programs served as the basis of the two-center integral input data of the final master energy band calculation program whose operation will now be summarized. Explicitly the basic input integrals

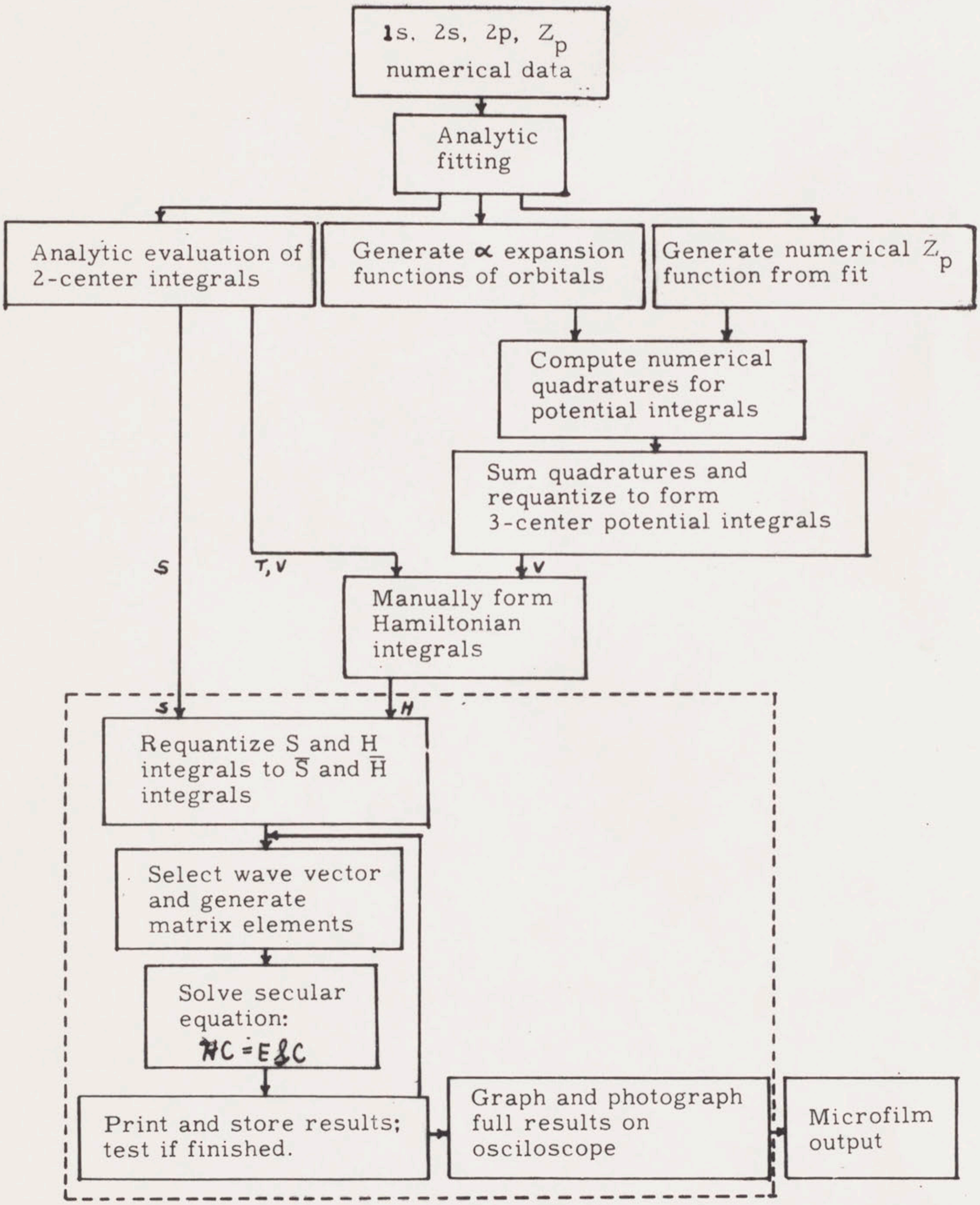


Fig. 6-1
Block Diagram of Computer Operations

were of the form

$$\overline{M}_{ij}(\vec{\rho}_a) = \int \psi_i^*(\vec{r}-\vec{\rho}_a)\,\mathcal{M}(\vec{r})\,\psi_j(\vec{r})\,dr \qquad (6\text{-}1)$$

where the ψ are atomic orbitals, $\vec{\rho}_a$ is the neighbor vector, and

$$\mathcal{M}(\vec{r}) = \left\{ \begin{array}{ll} \mathcal{S}(\vec{r}) = 1 & \text{, Overlap} \\ \mathcal{H}(\vec{r}) = -\frac{1}{2}\nabla^2 - \sum\limits_{\vec{\rho}_b} \dfrac{Z_p(\vec{r}-\vec{\rho}_b)}{|\vec{r}-\vec{\rho}_b|} & \text{, Hamiltonian} \end{array} \right. \qquad (6\text{-}2)$$

the sum in the potential term being over all neighbor vectors. In the present calculation, the three-center potential terms were neglected when $|\vec{\rho}_b|$ or $|\vec{\rho}_b - \vec{\rho}_a|$ exceeded the fourth-neighbor distance in the sum over $\vec{\rho}_b$.

The operation of the master energy band program then proceeded as follows. For a given value of the reduced wave vector, $\vec{k}$, the program computed the Hamiltonian and overlap matrix elements arising from the Bloch waves constructed from the atomic orbitals. These matrix elements were made real by taking judicious linear combinations of the Bloch waves as basis states, as was described in Chapter 2, and had the form

$$\mathcal{M}_{ij}(\vec{k}) = \sum_{\vec{\rho}_a} \pm M_{ij}(\vec{\rho}_a) \left\{ \begin{array}{l} \cos(\vec{k}\cdot\vec{\rho}_a) \\ \sin(\vec{k}\cdot\vec{\rho}_a) \end{array} \right. \qquad (6\text{-}3)$$

where the terms in which $\vec{\rho}_a$ exceeded the ninth-neighbor distance were neglected. The program next solved the usual variationally-derived secular equation of the form

$$\sum_{j=1}^{M} \mathcal{H}_{ij}(\vec{k})\, C_{j\ell}(\vec{k}) = E_\ell(\vec{k}) \sum_{j=1}^{M} \mathcal{S}_{ij}(\vec{k})\, C_{j\ell}(\vec{k}) \qquad (6\text{-}4)$$

and stored for later use the eigenvalues $E_\ell(\vec{k})$. A new value of the wave vector was then selected and the generation and solution of the secular equation repeated until the pre-set values of the wave vector were exhausted. This cycle of the wave vectors was done twice, once for the sequence of 8 by 8 secular equations arising from the σ states and once for the 2 by 2 secular equations of the π states. Finally for convenience, the program displayed graphically on a photographic oscilloscope cross-sectional views of both the σ and π energy bands, $E_\ell(\vec{k})$ vs. $\vec{k}$, for values of the wave vector along the edges of a basic non-repeating 30° - 60° - 90° triangle of the first Brillouin zone.

The solution of the secular equation was done by utilizing a Jacobi's method matrix diagonalization program in conjunction with standard matrix multiplication techniques. This solution process is described in detail in the memorandum, given as Appendix B, describing two general purpose secular equation utility programs which were by-products of the present calculation.

In view of the intimate application of a high-speed computer to the present calculation, it is worthwhile to discuss further some of the general conclusions which arose out of this experience. Perhaps the most difficult readjustment of mental approach required for machine computation versus the traditional desk calculator computation is taking proper account of the shift in usefulness of a modern computer. Although in the sense of arithmetic operations, a computer is an extrapolation of a desk calculator, because a computer must be given in advance a complete set of logical instructions which anticipate all contingencies, there is a sharp shift in the choice of useful applications. Thus a desk computer is valuable for non-systematic computations where there is a high degree of logical complexity with very few repetitions. Conversely the modern computer is at its best when doing very repetitious elementary logical steps on vast quantities of data.

A modern computer also presents a further complication which arises from the organization required to couple-together a series of programs which are equivalent to many steps of hand computation; at times in very complicated and large computer programs, this "juggling act", which increases in difficulty in a greater than linear way with the magnitude of program, severely taxes the concentration and memory for details of the programmer.

The great intensity of effort required by the programmer also aggravates a more personal problem associated with computer work. This problem is the all-or-nothing nature of a program and the accompanying personal involvement and frustration. The average large program, thanks to the capacity and versatility of modern computers, is usually an ambitious affair. Thus the typical computer program will involve many hundreds of instructions which at the first writing invariably will contain mistakes, sometimes of a clerical nature or, even worse, sometimes involving serious logical confusions, (a mistake per hundred instructions is low even with considerable programming experience). Clearly these mistakes have to be discovered and removed, a process often called trouble-shooting.

The programmer first plans out a testing procedure for the program which, if well-done, will test every contingency of the program operation. This often requires an organization and decomposition into many small test procedures which, in the end, results in another computer program rivaling the original program in difficulty and complexity. The trouble-shooting process then begins and the combined original program and test program are run on the computer. Since most mistakes result in logical absurdities which stop the computer, the test run usually fails to finish correctly. The programmer then infers from any partial test results he may have obtained plus the knowledge of how the program stopped what mistake among the hundreds of instructions involved might have precipitated the failure. If the programmer, after several hours of study, fails to find the mistake he must, of course, back-up and make a more detailed test run so as to have additional information for inference. When he is successful in finding his mistake, he then makes a correction and repeats the trouble-shooting process until after many runs he is finally able to get the entire program tested.

Besides the uncertainties of how many mistakes a program will contain, (stoicism is an asset), the trouble-shooting process is aggravated by the necessarily cooperative-nature of a machine computation center. Thus all computing machines, in order to be efficiently operated, must not only be used by several dozen programmers but also must have priorities and scheduled running times. This invariably results in delays ranging from several hours to several days before a partially tested program can be corrected and rerun.

From the previous discussion of the trouble-shooting process and scheduled operation of computers it is clear that the use of a modern computer bears considerable resemblance to the use of nuclear reactors, cyclotrons and other large experimental devices. At the present time there is no escaping the fact that it is very difficult to use a digital computer casually, although, the current evolution of programming techniques is improving this situation. An indication of the current status of programming technique is the rule-of-thumb that computations which require less than one to three months should still be done with a desk computer.

Turning from general remarks, the magnitude of programming in the present calculation was quite large. Roughly speaking this programming was split into two major parts: the evaluation of the two- and three-center integrals and the generation and solution of the energy band secular equations. At the start of the present calculation it was hoped that two-center integrals would suffice and that in the matrix element generation not many neighbor distances, (0, 1, 2, and 3), would have to be considered. Thus the programs for two-center integrals, described in Chapter 3, and a secular equation generation and solution program were written. Upon obtaining energy band results from these programs, both programs were found to be inadequate;, crude estimation of three-center integrals indicated an important effect being omitted and the failure of the overlap matrix to be positive definite, (i.e. have positive definite eigenvalues), at certain wave vector values revealed that several more neighbor distances were required for accurate overlap matrix elements.

These failures forced the calculation from the initially moderate amount of programming to the rather large and lengthy final form. It was necessary to completely revise the secular equation generation and solution program so as to have the additional neighbor distance generality required. In addition the rather elaborate energy band display program was devised for the convenience of rapid interpretation of the band structures.

The three-center integral procedures also required new programs since the method had not been applied before on the Whirlwind computer. Because of the generality of the method used for these integrals, two utility programs, the expansion function generation program and the numerical quadrature program, were written with special care given to flexibility and ease of application; hindsight has shown that such care was quite justified since these programs have been instrumental in lightening the labor of the integral evaluations required by several other members of the Solid-State and Molecular Theory Group.

From the above remarks, it can be seen that there were two major difficulties in the present calculation. First there was an underestimation of the scope of the computation required for meaningful solutions. In a certain sense this difficulty represented a result in itself since it gave quantitative information concerning the application of the tight-binding method to crystals. In any case there are always some magnitude uncertainties in research work involving numerical methods although careful preliminary estimation can minimize one's efforts. The second difficulty involved the unavailability of the machinery for the two- and three-center integrals and the subsequent programming. Because such programs have general interest in molecular structure studies, it seems clear that they ultimately can be developed into relatively standard forms so that computations similar to the present one will be greatly simplified in the future.

The uniqueness of the Whirlwind I computer also had an effect on the present calculation. In particular, too many mathematical functions were not available in adequate program form. Thus because of unreliability, poor efficiency or unavailability, it was necessary to write and test programs for generating many functions, (e. g. $i_n(x)$, $k_n(x)$, e^x, $C_n(x)$, $B_n(x)$, $F_\ell^{mm'}(\beta)$). The experience gained as a Research Assistant in Numerical Analysis and Machine Computation was especially valuable for this purpose. It is to be hoped that in the future as computing machines become more standardized that a large stock of function generation programs will become available as a result of the efforts of many programmers.

Finally it is of interest to note some of the deficiencies in the final programs for this calculation. The secular equation generation program could have been more general in two ways. First, it would have been desirable to have the possibility of including more excited Bloch wave states, or perhaps even better, including excited plane wave states (i. e.

essentially developing a modified orthogonalized plane wave method). These additional basis states would then allow one to test the accuracy of the valence electron energy band solutions, which in a mathematical sense only depend on the original choice of the crystal potential. Second, it would have been very desirable to have been able to treat the three-dimensional graphite band structure, with its corresponding 20 by 20 secular equation, by simply including more integral values. The factorization which was made into σ and π energy bands is no longer considered very useful in a calculation of the present complexity since the programming was necessarily more complicated and the machine time saved was negligible.

To accomplish these two improvements in the secular equation generation, it is strongly felt that systematic matrix techniques should be introduced wherever possible and that the geometry requantizations and sign convention difficulties should be minimized by use of the $F_\ell^{mm'}(\beta)$ function discussed in Chapter 5. The use of such techniques in a program would simplify the writing and testing and minimize the possibility of an error.

In an attempt to summarize the remarks of this chapter, it is felt that a considerable part of the computational effort in the present work was spent on the more general problem of efficiently utilizing a modern digital computer. Since the latter problem is of considerable complexity, most computing centers have a group of staff members who prepare useful programs for general use. On the basis of the needs of the present calculation, it would appear that these programs fall into three categories: specialized problem programs, subroutine programs, and utility programs.

Considering the specialized problem programs, examples are the generation of the atomic orbital expansion functions and the two-center integral programs. This type of program is usually quite complex and limited in application to a specific field of research. Consequently the development of these programs will probably receive low priority by computer staff members and will have to be done by computer-experienced research workers of the various fields.

Subroutines are the most valuable prepared programs in computer work since they represent mathematically closed problems. Thus, the input and output data of these programs is succinctly stated in mathematical terms. Examples of these programs are function generation, matrix diagonalization and numerical integration. Because of the wide-spread applications of subroutines they are best developed by the more experienced computer staff.

Utility programs are defined to be programs which accomplish one or more mathematical operations with very simple directions and with virtually no programming required. Excellent examples of this type of program are the secular equation utility programs described in Appendix B. Utility programs are made up usually of one or more basic subroutines but have the essential difference that no programming is required to operate the subroutines nor to take the results out of the machine. Present experience with the secular equation and numerical quadrature programs has indicated that utility programs can greatly speed up the process of using a computer, even for an experienced programmer. As with the subroutines, these programs can be prepared by computer staff members.

Thus it is clear that a great deal of standard programming can be done in anticipation of general computer use. The gradual development of the ease of computer applicability is still growing so that as yet there is no limit to the complexity of the computational problems which will be solved in the future, although drastic improvements over present computations would appear unlikely.

Chapter 7

Results and Conclusions

A physically significant result in a two-dimensional energy band calculation of graphite is the size of the gap between the five lowest (occupied) and the higher (excited) σ bands, and in particular whether or not the two lower π bands (valence and conduction), which are degenerate at one value of the wave vector, have their point of degeneracy in the σ band gap. If such a σ band gap is large enough to include all of the π bands, then it follows from perturbation theory that a reasonable approximation for computing the conduction properties of a three-dimensional graphite would be to ignore the σ states; (as pointed out earlier, the σ and π are no longer "good" symmetry designations in the three-dimensional crystal since the σ and π Bloch waves of alternate graphite layers interact, but the terminology is still used.)

A second result of this band calculation which is of interest is the width of the occupied bands formed from the Bloch waves of 2s and 2p atomic orbitals. This width is directly comparable with the energy width of the soft X-ray emission spectra of the graphite valence band which has been obtained by Chalkin[25]. As estimated by Coulson and Taylor[5] the experimental width is about 15 e.v. although examination of the data curve indicates a possible latitude of a few electron volts more or less.

The energy band solution of the present calculation is shown in fig. 7-1 where the horizontal dimensions are the edges of the basic triangle of the first Brillouin zone as shown in fig. 2-3. Energy values of interior points of the triangle were also found and are included in Appendix D which gives the complete numerical results. These interior energy bands vary smoothly from the edge band values so that they are only included in the numerical tabulation of the results given in Appendix D. In addition, the two lowest σ bands, which arise almost entirely from the Bloch waves of 1s atomic orbitals, are omitted from fig. 7-1 since the bands are nearly independent of the wave vector and at an average value of -15.75 Rydbergs. Finally fig. 7-2, which is the same as fig. 7-1 except for a partially coarser mesh of wave vector values, is the output of the master energy band calculation computer program.

From fig. 7-1 it is observed that the highest occupied point in the sigma bands occurs at pt. O, ($\vec{k} = 0$), with a value of +.430 Rydbergs. The lowest excited σ band has roughly a constant minimum value for wave vector values forming an approximate circle about pt. O, the minimum value being about +1.158 Rydbergs. The degeneracy point of the bands falls at +.570 Rydbergs, a value representing the Fermi level for zero temperature. Thus it is clear that these results support to some extent the usual approximation of neglecting the σ states in calculations of graphite conduction properties, which depend on the nature of the energy bands in the vicinity of the Fermi level. However,

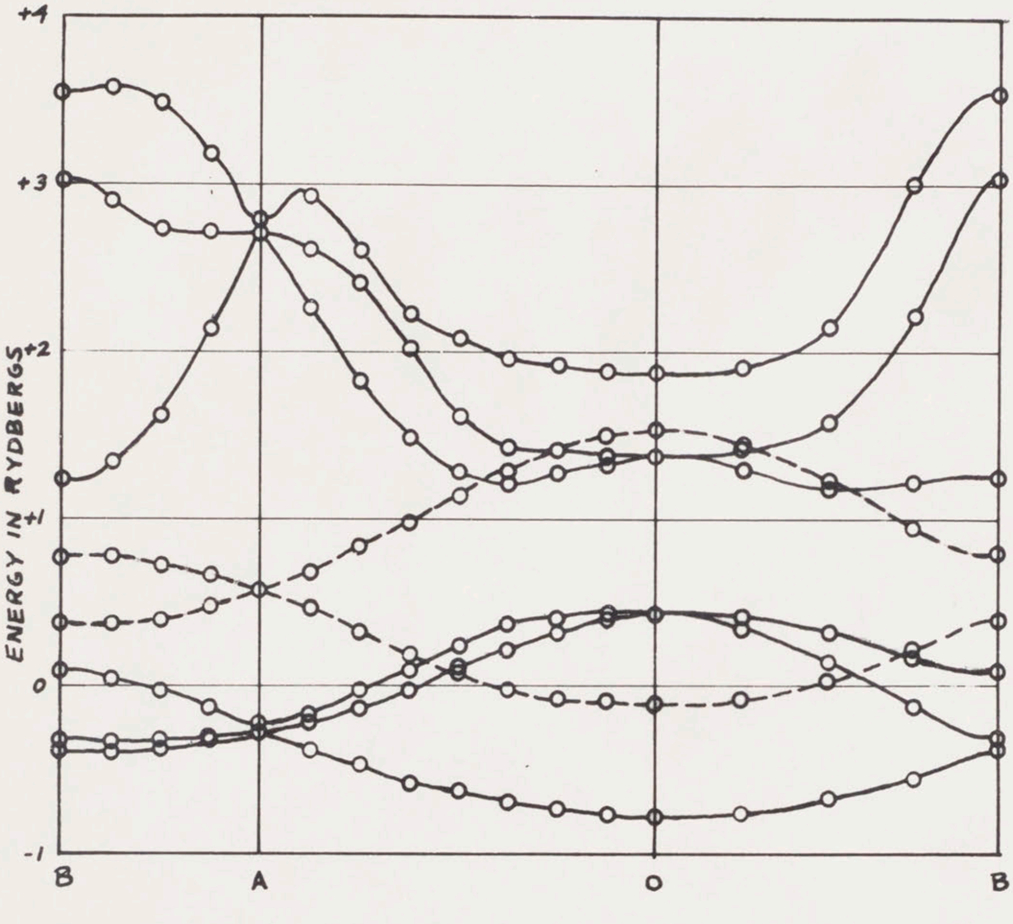


Fig. 7-1

Two-Dimensional Graphite Energy Bands

—— = σ bands

– – = π bands

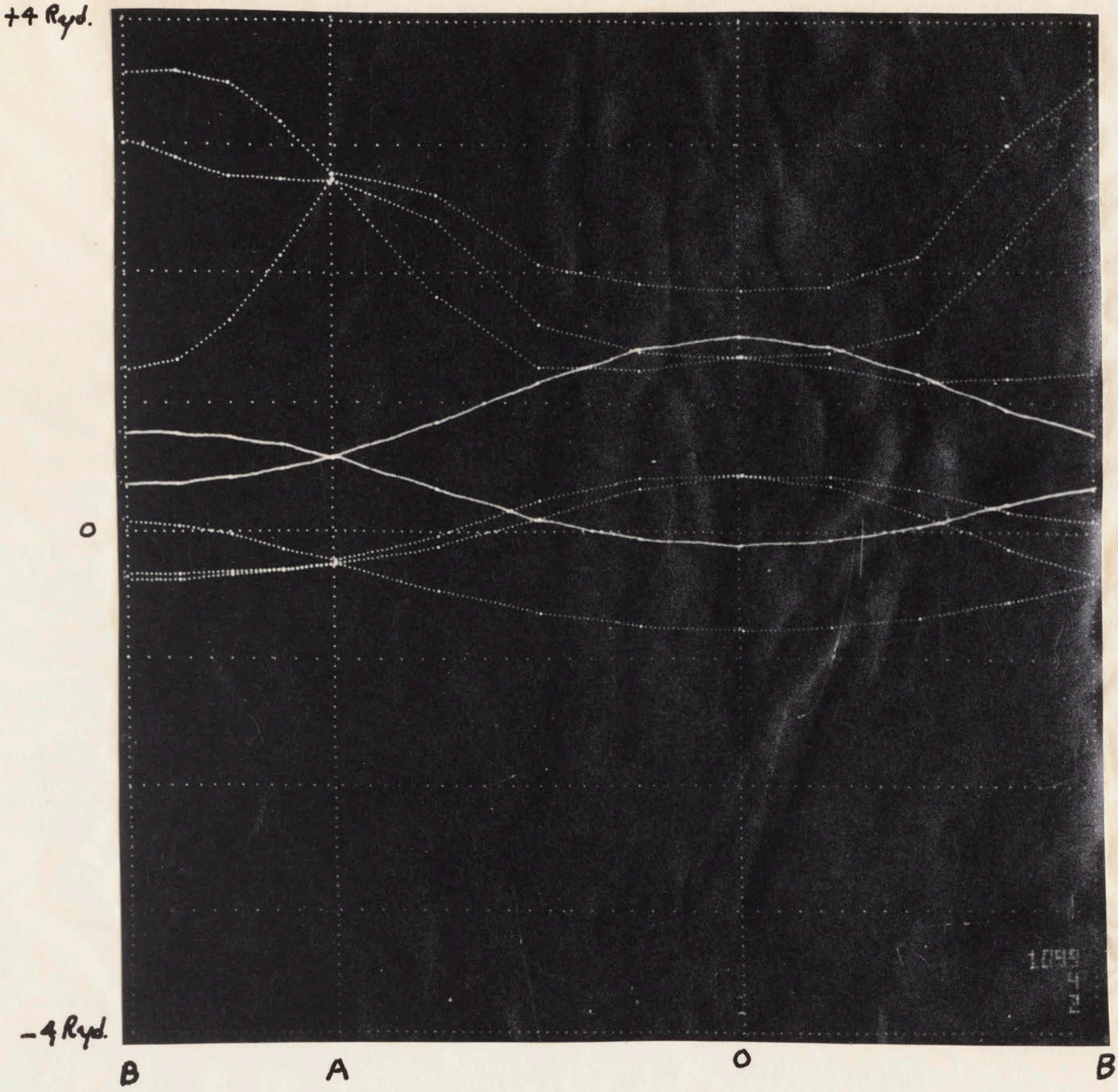


Fig 7-2
Two Dimensional Graphite Energy Bands (Code No. 1099)

this calculation shows by virtue of the overlapping of the σ and π bands that for a cohesive energy calculation, which depends on energy values for all wave vectors of the Brillouin zone, the σ states must be included.

The bottom of the σ band in fig. 7-1 occurs at pt. O with a value of $-.787$ Rydbergs; thus the width of the calculated valence band is 1.357 Rydbergs. This value corresponds to 18.5 e.v. which is in good agreement with the approximate experimental width of 15 e.v.

Consideration can also be made of the potential function used in the present calculation. The potential, which was formed by superpositions of the $\frac{1}{r}Z_p$ function, clearly omits exchange effects. Slater has given a procedure for introducing an approximate exchange potential correction within the framework of the one-electron approximation[26]. This exchange potential correction, if applied, would be proportional to the cube root of the charge density of the occupied crystal wave functions. Consequently, one would expect the occupied bands to be lowered more in energy than the unoccupied bands since the unoccupied wave functions are orthogonal to the occupied wave functions. Thus, it is plausible that a more careful consideration of exchange effects in the present calculation would only broaden the σ band energy gap and would leave the present results qualitatively unchanged.

One of the more striking features of the present results is the smoothness of the energy bands. In fact, these bands are similar to those obtained from the Slater and Koster interpolation procedure wherein the tight-binding method is used with neglect of all but a few nearest-neighbor integrals[8]. An example of this interpolation is given in fig. 7-3 where the overlap matrix was assumed to be a unit matrix and the effective Hamiltonian integral values are those obtained by Slater and Koster with an empirical fit at symmetry points of diamond energy bands. The Hamiltonian integral values used are given in Appendix C.

Because of the rough similarity between the present calculation and the interpolation example, it is of interest to examine the stability of the present results in view of the several possible simplifying approximations.

Omission of the 1s Bloch waves was found to have an overall lowering and warping effect on the σ bands in such a way that the σ band gap was roughly reduced by half. This modified solution is shown in fig. 7-4.

This result indicates that the σ states formed from 2s and 2p atomic orbitals were seriously non-orthogonal to the 1s Bloch waves. The variation in the size of the gap shows especially that meaningful results cannot be obtained without inclusion of the 1s Bloch waves.

A second possible approximation made was the omission of all the three-center potential integrals. This left the π bands nearly the same but made a very pronounced change in the σ bands, again closing the σ band gap down to

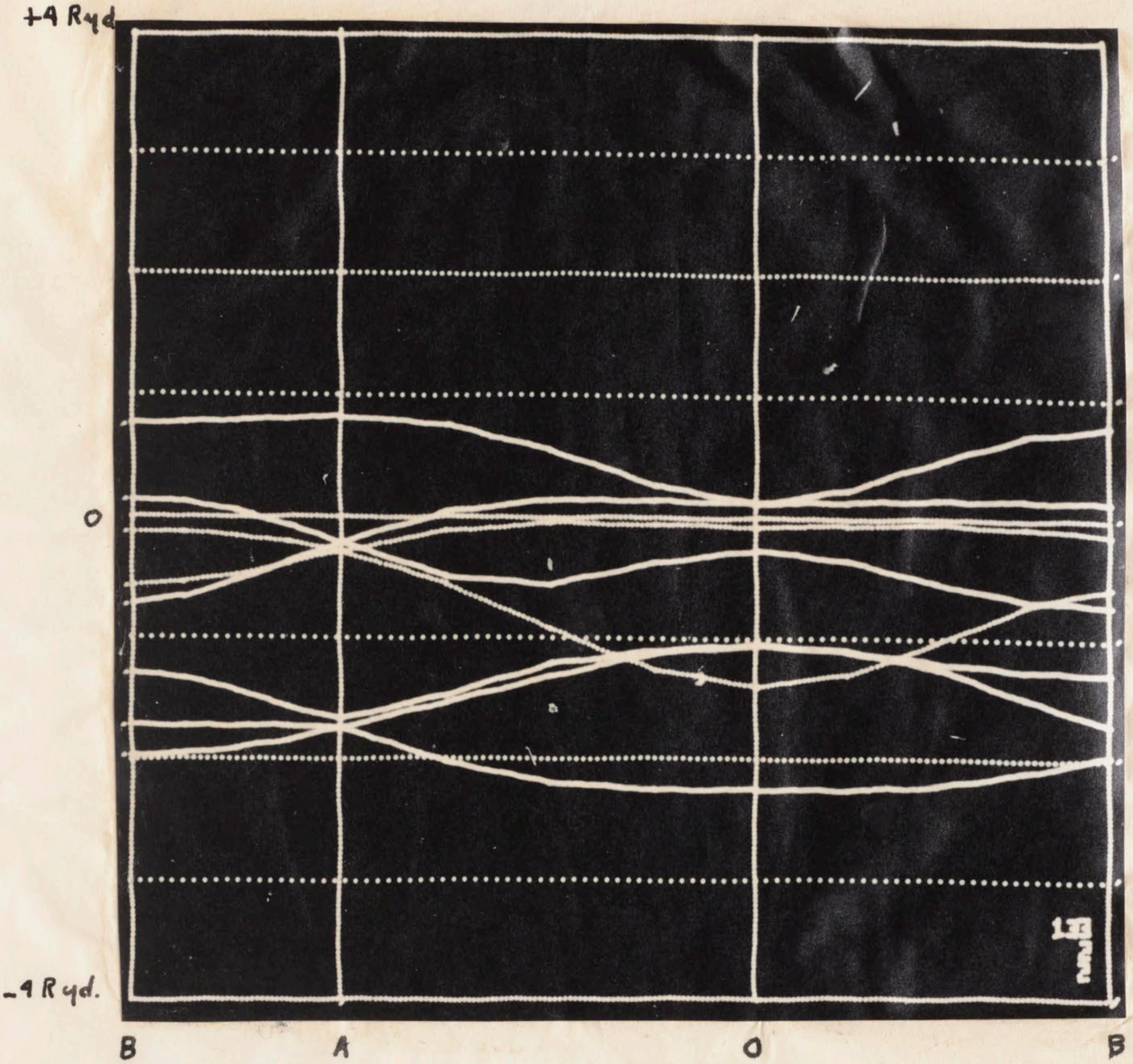


Fig. 7-3
Graphite Energy Band Interpolation
Example with Diamond Integral Values
used (Code No. 133)

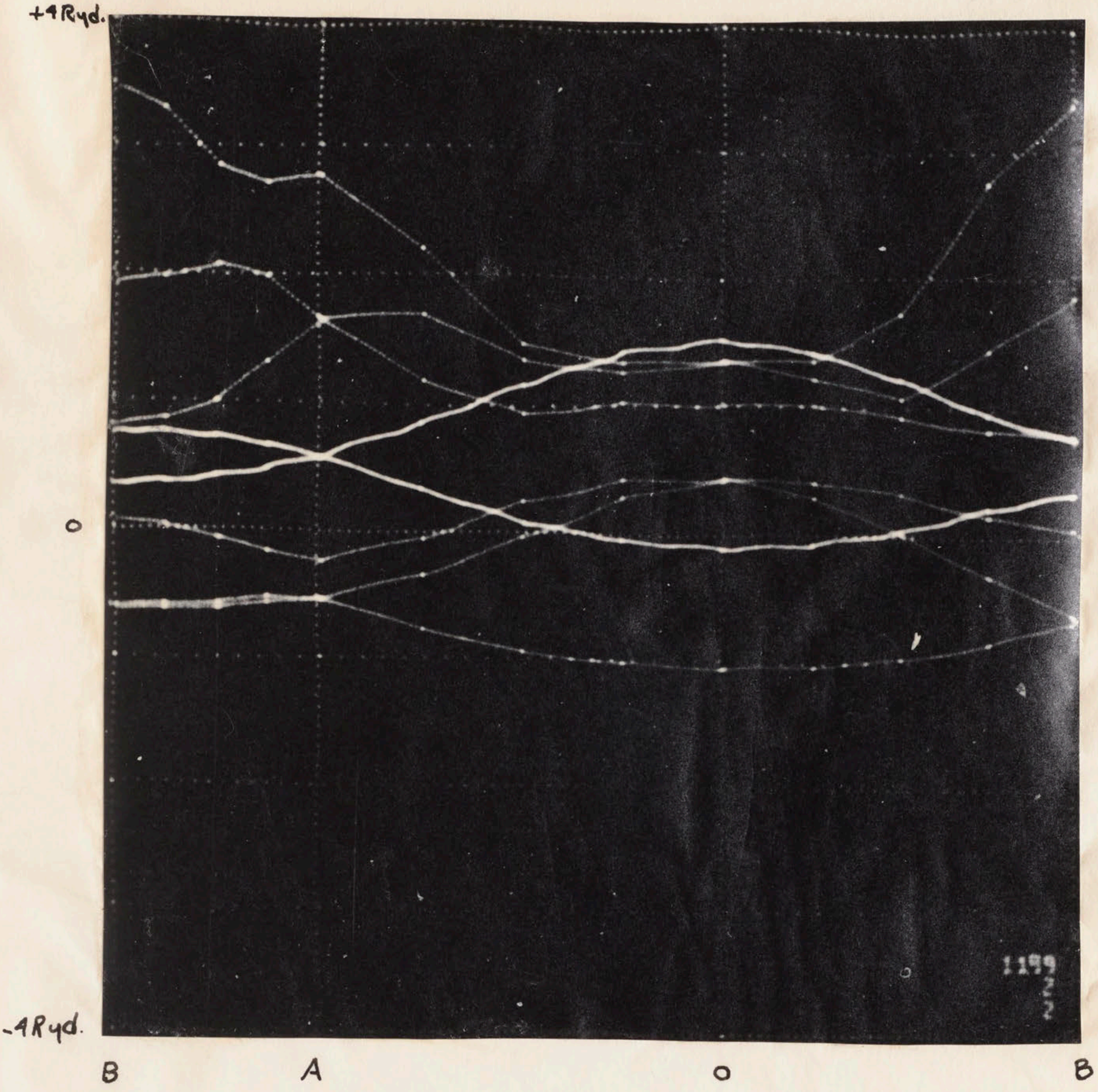


Fig. 7-4

Energy Bands (Code No. 1199)

1s Bloch Wave States omitted

about half but also lowering the gap so far that the π band Fermi level no longer was included. Fig. 7-5 illustrates this solution. The altered Hamiltonian integral values are given in Appendix C. It should be noted that the integrals used to give the results of fig. 7-5 were obtained by the methods of chapter 4 before the machinery of chapter 5 had been prepared. Thus the two-center potential integrals differ slightly from those used for the results of fig. 7-1. However, these discrepancies are not meaningful since they affect the accuracy of the matrix elements less than the exclusion of the three-center potential integrals.

Finally the solutions were examined with respect to the approximation of omitting the higher neighbor distance integrals in the generation of the secular equation matrix elements. The stable solution (fig. 7-2), which included up to ninth neighbor distance integrals, was graphically unchanged when only up to eighth neighbor distance integrals were included (fig. 7-6), so it is clear that all the matrix element series had converged. The solution was found to be only slightly warped when only up to fifth neighbor distance integrals were included in the σ bands and when only up to third neighbor distance integrals were included in the π bands. The solution including up to fifth neighbor distance integrals is shown in fig. 7-7 and the solution including up to third neighbor distance integrals is shown in fig. 7-8. As is seen in these figures, truncation of fifth or less neighbor distance integrals in the σ bands caused large

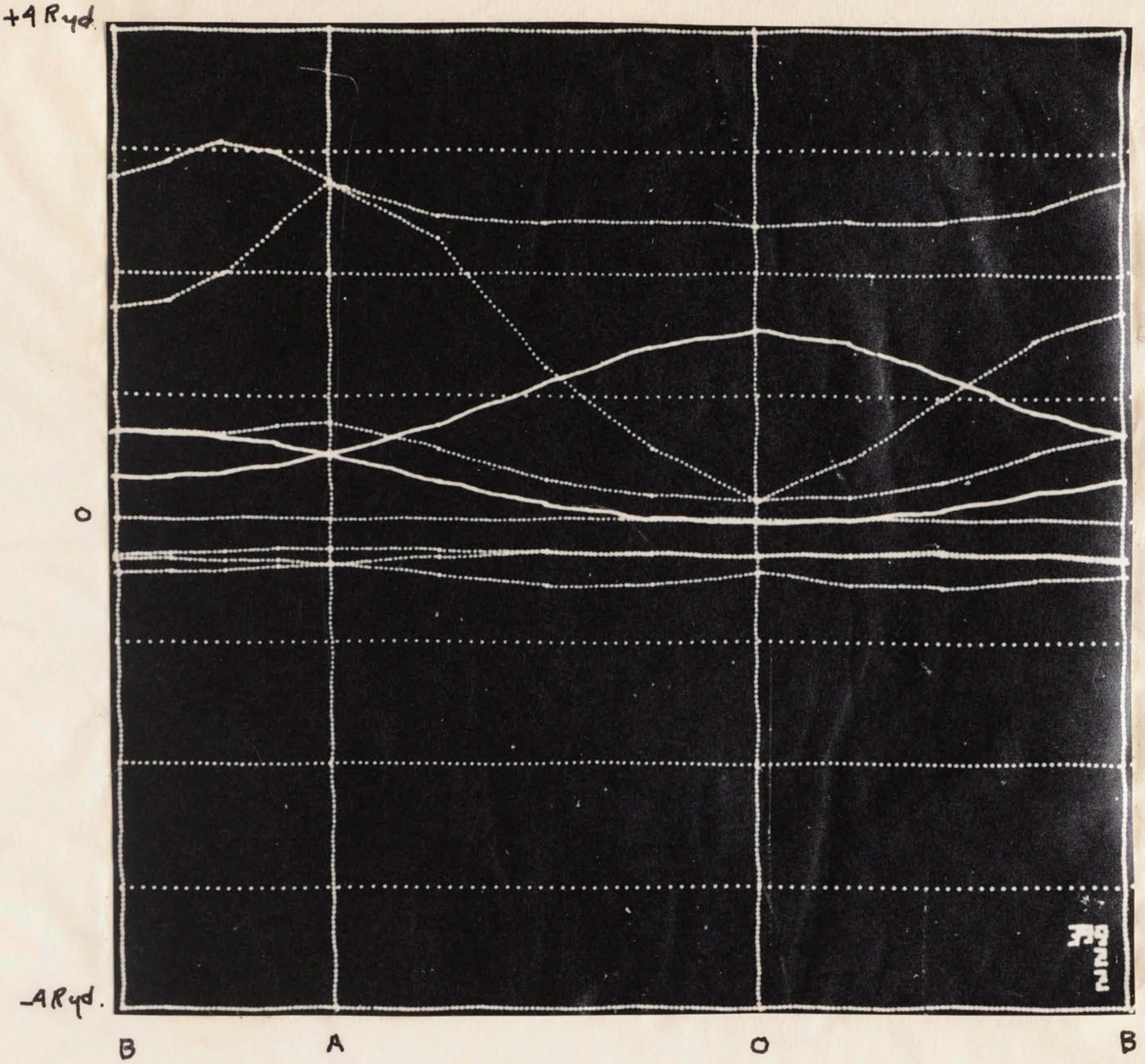


Fig. 7-5

Energy Bands (Code No. 399)

Three-Center Potential Integrals omitted

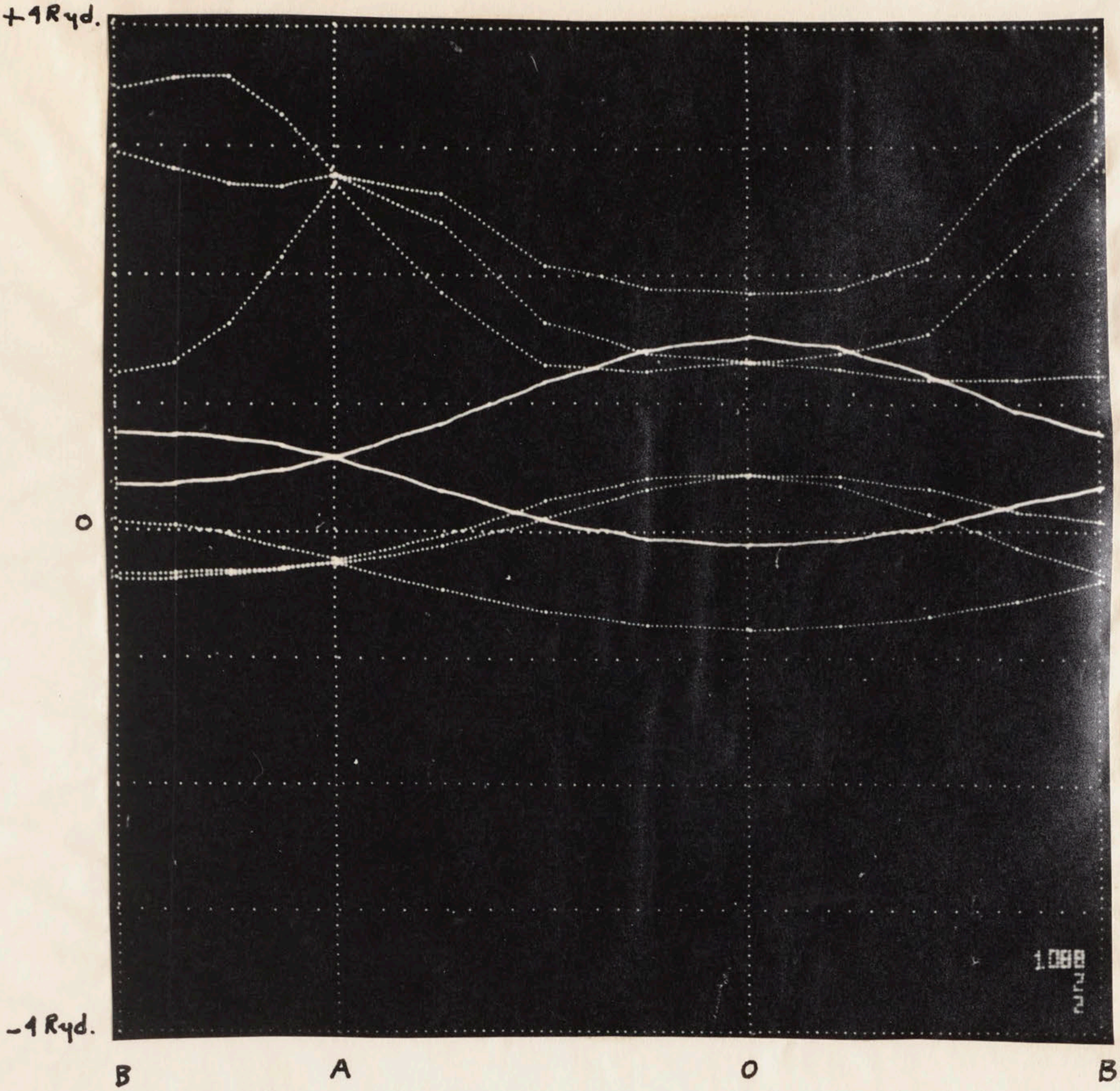


Fig. 7-6
Energy Bands (Code No. 1088)
Ninth Neighbor-Distance Integrals omitted
in Hamiltonian and Overlap Matrix Elements

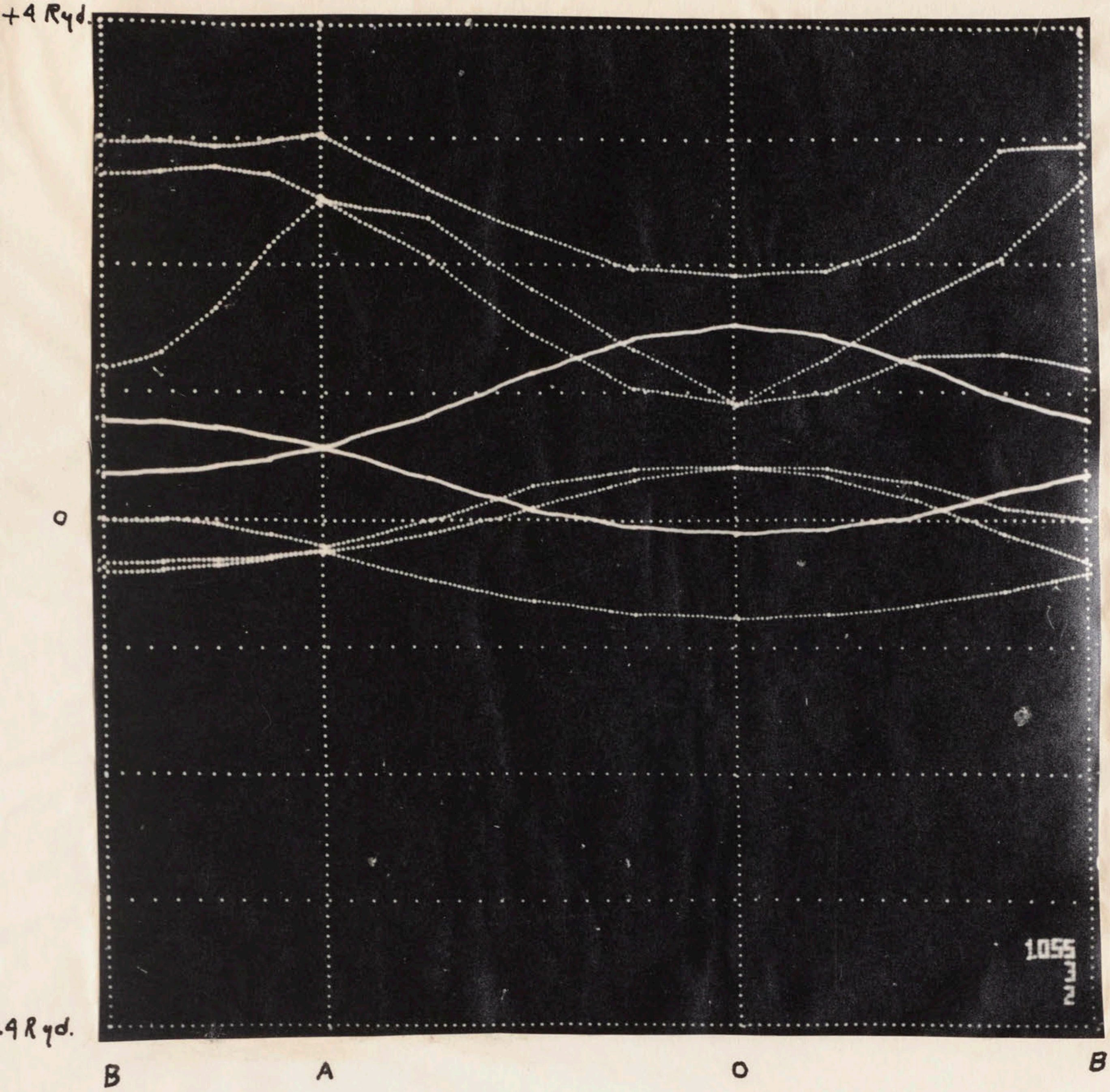


Fig. 7-7

Energy Bands (Code No. 1055)

Sixth and Higher Neighbor-Distance Integrals omitted in Hamiltonian and Overlap Matrix Elements

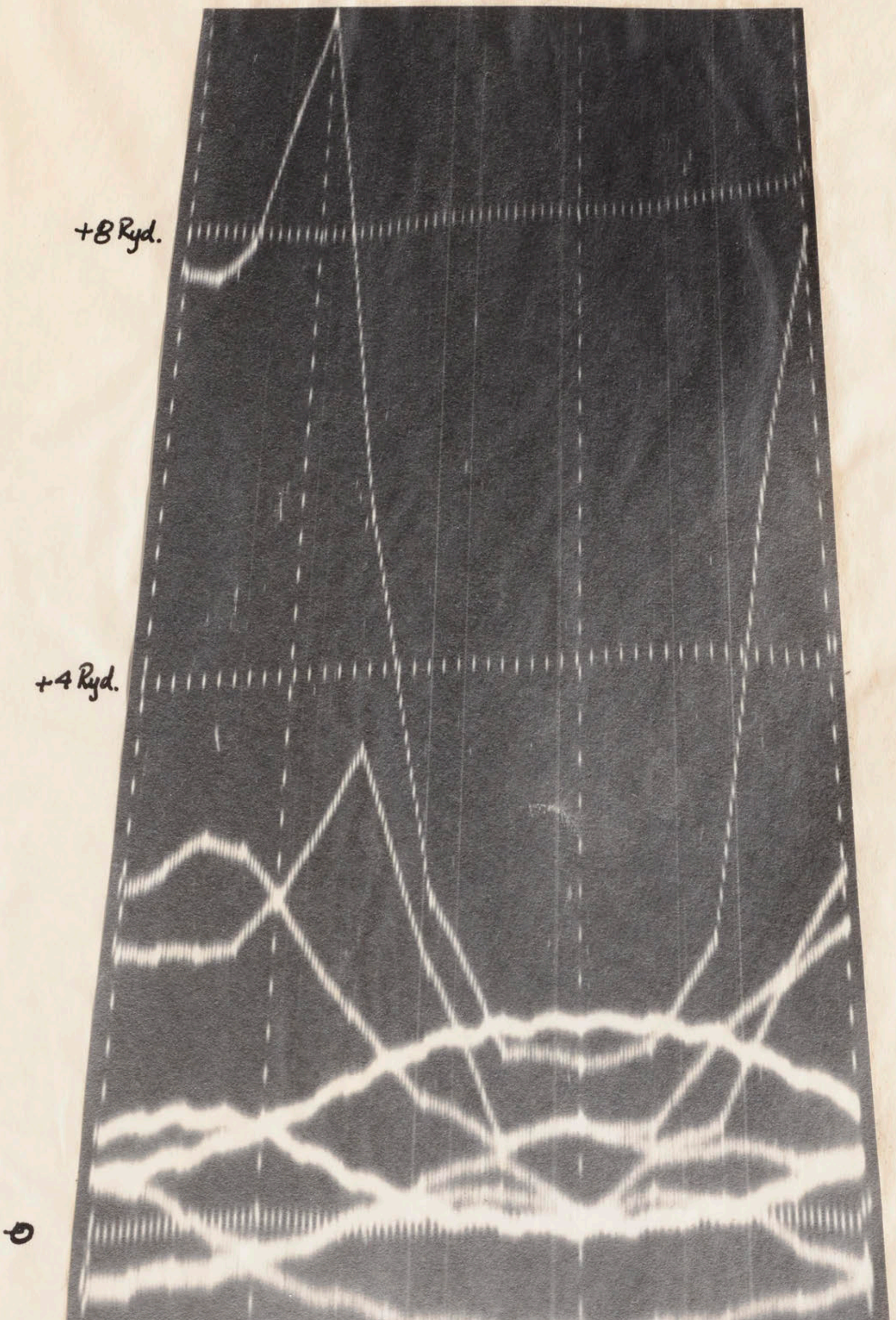


Fig. 7-8
Energy Bands (Code No. 1033)
Fourth and Higher Neighbor-Distance Integrals omitted
in Hamiltonian and Overlap Matrix Elements

changes. It is for this reason that the numerical calculation made by Lomer[6], which included only zero and first neighbor distance integrals, is not believed to be valid.

In addition the effects of truncating only Hamiltonian or only overlap neighbor distance integrals were investigated. It was found that the solution was sensitive to both Hamilitonian and overlap neighbor distance truncation to roughly the same extent and that the two effects were essentially additive. Figures 7-9 and 7-10 indicate the effects of truncating the Hamiltonian integrals after the fifth and third neighbor distances, respectively; figures 7-11 and 7-12 indicate the effects of truncating the overlap integrals after the fifth and third neighbor distances, respectively.

Thus the results of all the approximation tests indicate clearly that the tight-binding method when used in a non-empirical way must be carried out with considerable mathematical rigor in order that a meaningful solution will be obtained. Furthermore, when the effect of a Slater exchange correction potential is considered, it is seen that the present convergence problem in the matrix element generation would have been even worse since this correction potential is more extensive as a function of r than the $\frac{1}{r}Z_p$ function which was used. Thus the integrals required would have fallen off very slowly with increasing neighbor distance.

There remains to consider the future prospects of the present calculation. Probably the most interesting extension

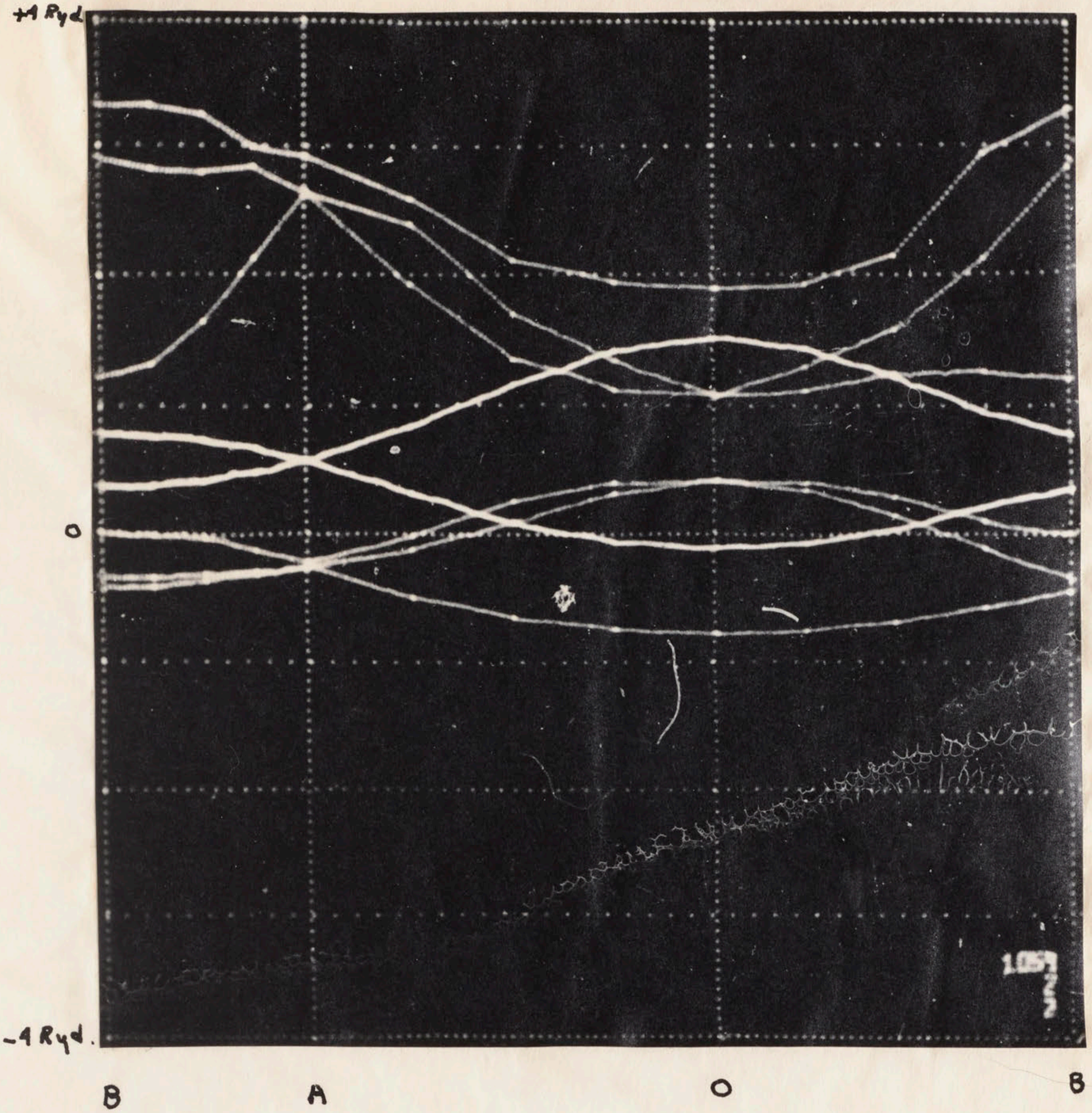


Fig. 7-9
Energy Bands (Code No. 1059)
Sixth and Higher Neighbor-Distance Integrals
omitted in Hamiltonian Matrix Elements

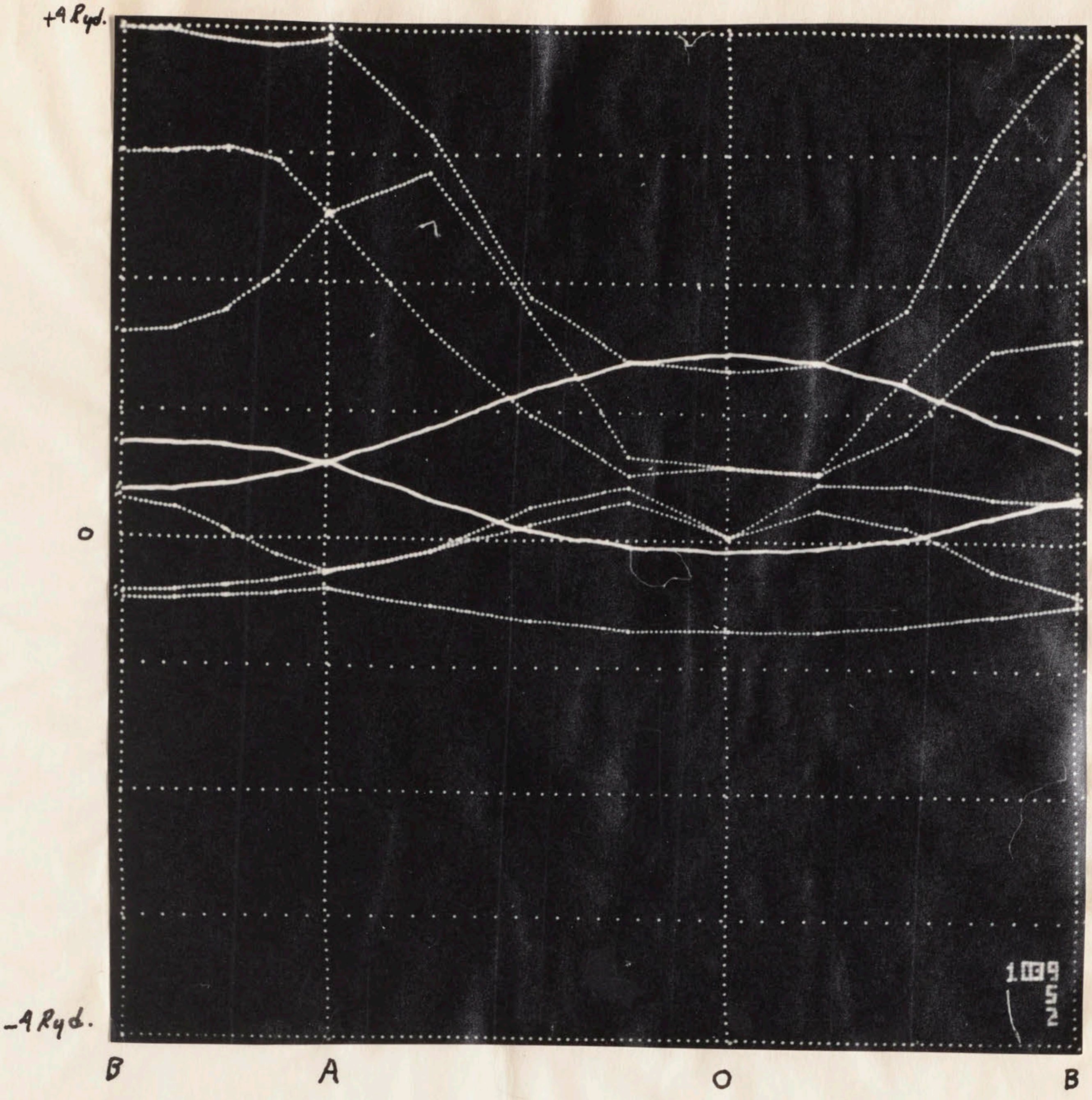


Fig. 7-10
Energy Bands (Code No. 1039)
Fourth and Higher Neighbor-Distance Integrals
omitted in Hamiltonian Matrix Elements

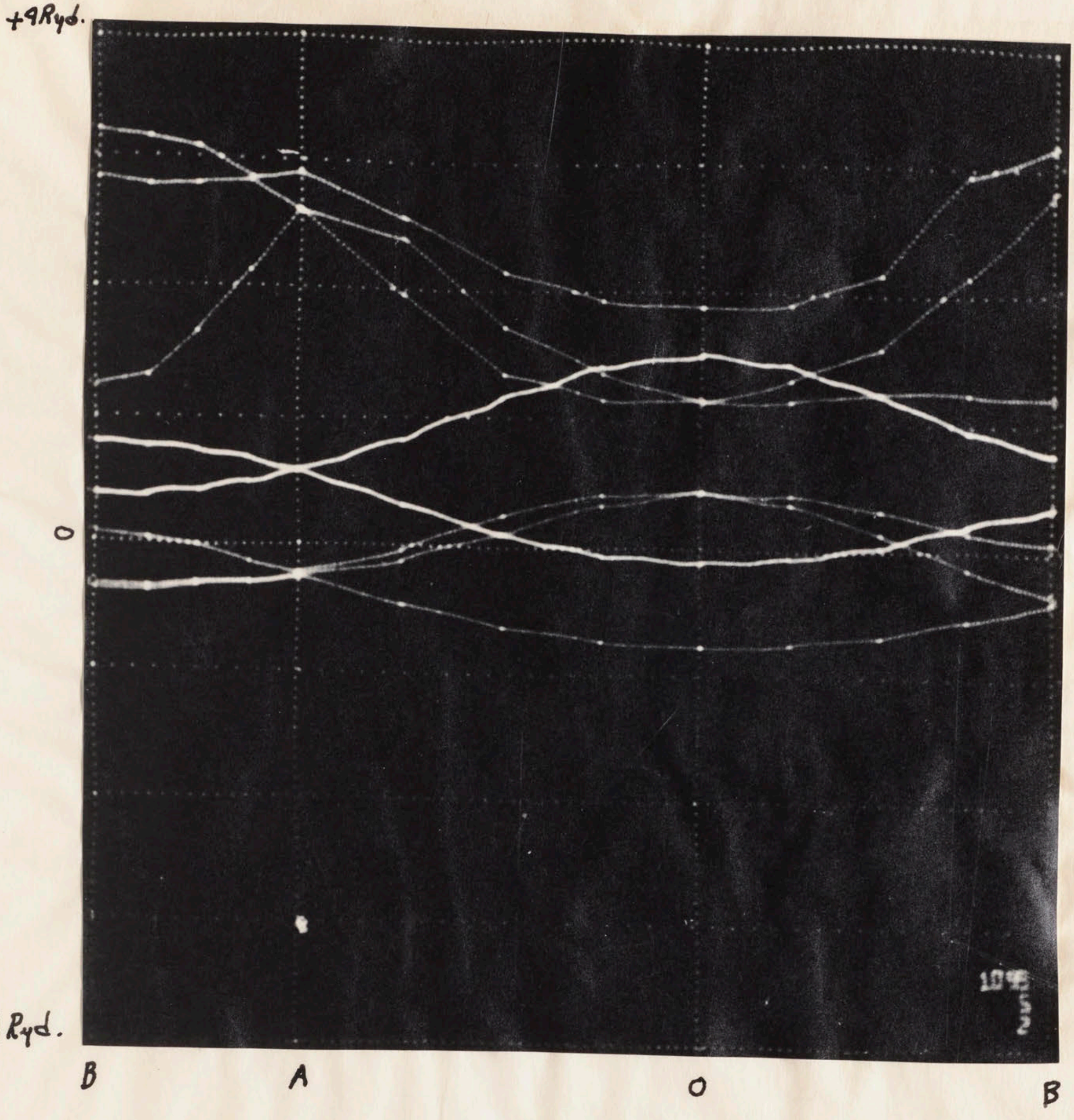


Fig. 7-11
Energy Bands (Code No. 1095)
Sixth and Higher Neighbor-Distance Integrals
omitted in Overlap Matrix Elements

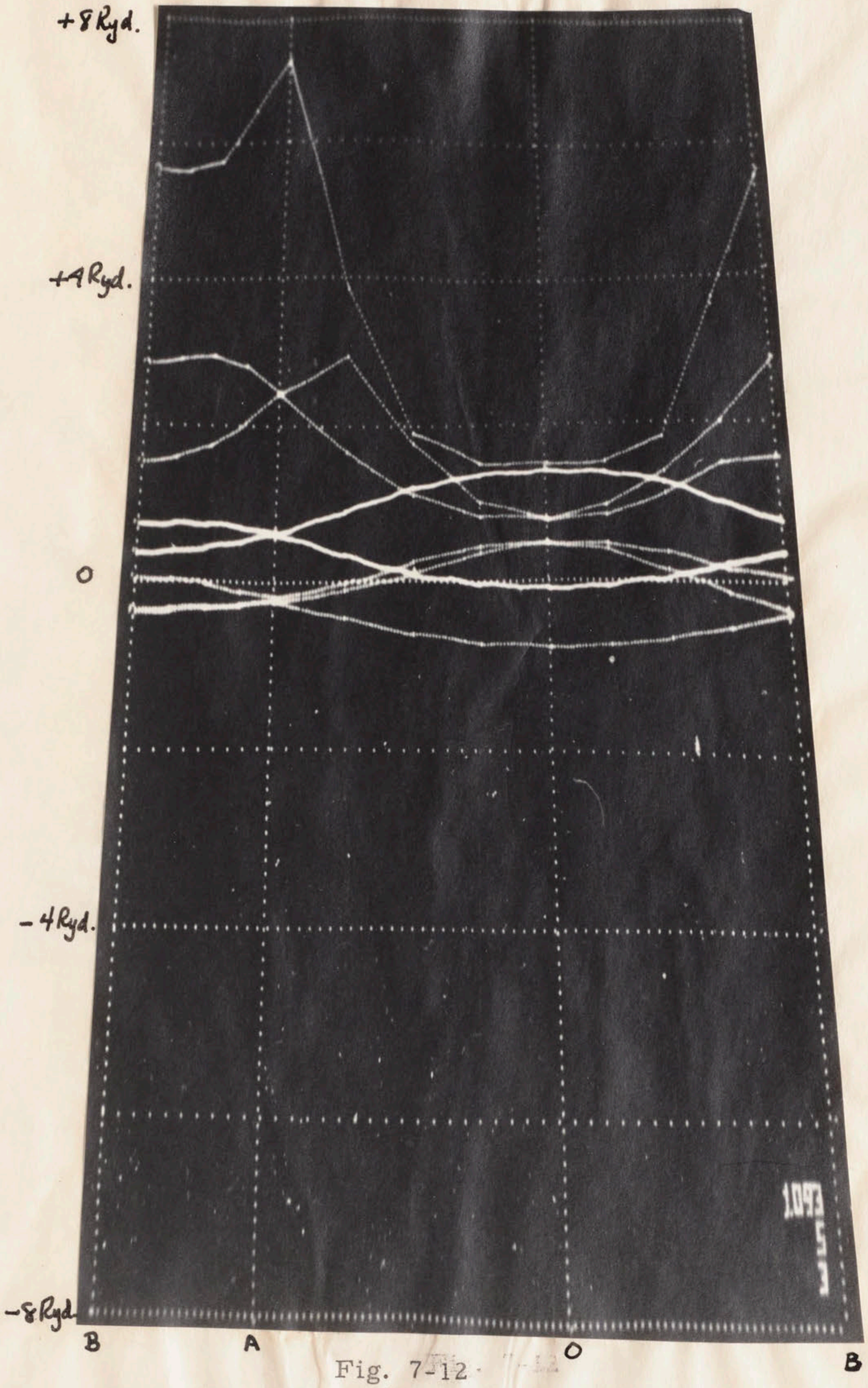


Fig. 7-12

Energy Bands (Code No. 1093)

Fourth and Higher Neighbor-Distance Integrals omitted in Overlap Matrix Elements of the work would be to solve the full 20 by 20 secular equation arising from the same wave functions in a three-dimensional graphite crystal. It is felt that the additional required integral values could be obtained by interpolation of the already known integral values given in Appendix C. The major part of such a calculation would be the computation of the wave vector dependent matrix elements and, unfortunately, the present computer program for this is not readily generalized. The procedures to write a new program were already discussed in chapter 6.

The most comparable calculation to the present one is the two-dimensional graphite calculation of Lomer[6], where he factorized the secular equation by group-theoretical methods at the three symmetry points, (O, A and B of fig. 7-1), and used only zero and first neighbor distance integrals to form the low-order secular equation matrix elements. For easy comparison, Lomer's results, which only include the four occupied valence bands, have been replotted in figs. 7-13 and 7-14. The zero of energy has been readjusted in these figures so that the lowest σ band at point O agrees with the corresponding value of fig. 7-1. The bands of fig. 7-13 were based on the assumption that the first neighbor integrals used to form the matrix elements obeyed the relation $H_{ij}(\vec{\rho}_\nu) = (-16 \text{ e.v.})\, S_{ij}(\vec{\rho}_\nu)$. The bands of fig. 7-14 were based on the assumption that $H_{ii}(\vec{\rho}_\nu) - H_{ii}(0) S_{ii}(\vec{\rho}_\nu) = \gamma = -3 \text{ e.v.}$. In both cases estimations were made for the remaining unspecified Hamiltonian integrals and the over-

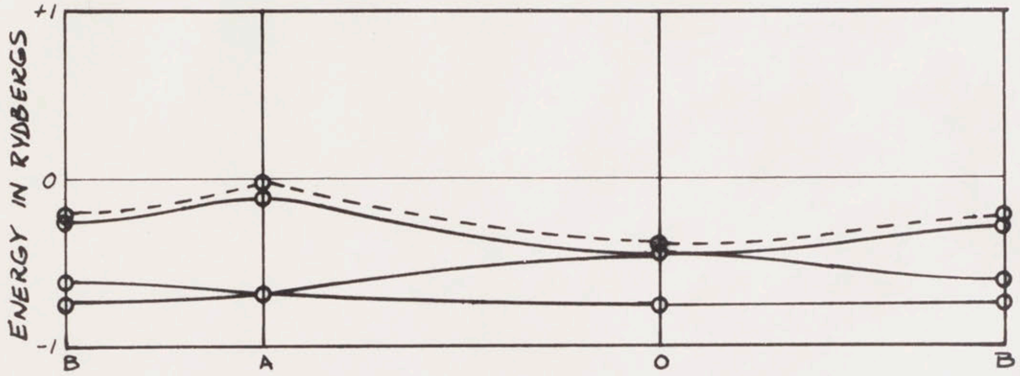


Fig. 7-13

Replot of Lomer's "fig. 4a" with zero of energy adjusted for comparison with fig. 7-1

—— = σ bands

– – = π band

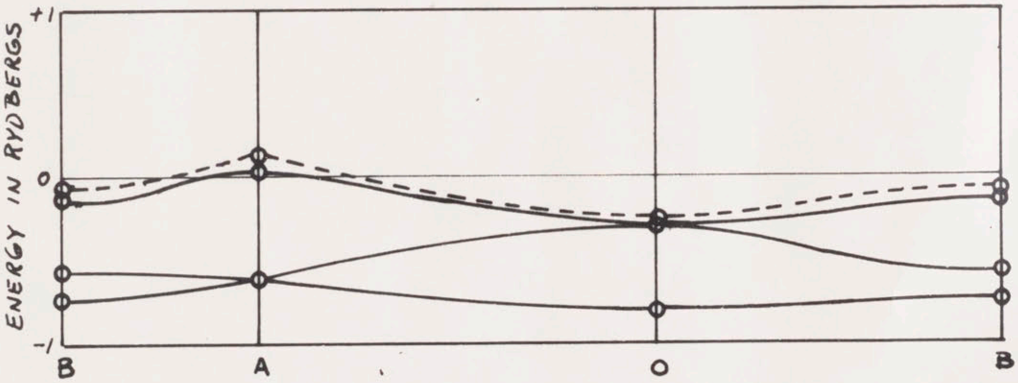


Fig. 7-14

Replot of Lomer's "fig. 4b" with zero of energy adjusted for comparison with fig. 7-1

—— = σ bands

– – = π band

lap integrals were obtained from nodeless Slater AO's.

At first glance the bands of figures 7-13 and 7-14 are similar to those of figure 7-1 with the ordering of the bands being nearly the same, the only exception being the inversion of the lower π and the doubly degenerate σ bands at point O, Closer inspection shows, however, that with respect to the present work, the energy values differ considerably and that the bands, which are of a total width of 10 to 12 e.v., are flatter. Moreover, the present calculation shows that many more neighbor distance integrals than Lomer used are required for meaningful convergence of the secular equation matrix elements. Thus if Lomer had included, for example, second neighbor distance overlap integrals, his results would have been quite different. Consequently Lomer's results must be viewed as an application of the Slater and Koster interpolation scheme where the effective integral parameters were obtained by qualitative arguments.

In summary, the present two-dimensional graphite calculation, by virtue of the σ band energy gap enclosing the π band degeneracy point, supports the usual approximation of using only the π states to study the vicinity of the Fermi level in three-dimensional graphite. The present results are also consistent with the experimental width measured for the graphite valence band. Finally the calculation demonstrates that very few approximations are legitimate in a tight-binding calculation of graphite and yet the results resemble those obtainable from the Slater and Koster interpolation scheme, which requires but a few parametric effective integral values.

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Biographical Note

Fernando José Corbató was born July 1, 1926 at Oakland, California, the first of two sons of Hermenegildo and Charlotte Corbató. In 1931 his family moved to Los Angeles, California, where he attended Selby Elementary School, Emerson Junior High School, University High School and in September 1943 entered the University of California at Los Angeles. A war-time enlistment in the U.S. Navy on May 15, 1944 served to interrupt his studies. After two years of training and experience as an electronic technician in the Navy he was honorably discharged on June 7, 1946. In September 1946 he entered the California Institute of Technology where he received in June 1950 a B.S. degree with honor standing. Since September 1950 he has been a graduate student at the Massachusetts Institute of Technology where he has held the positions of Teaching Assistant (1950-51), and Research Assistant in Numerical Analysis and Machine Computation (1951-56).

The honorary and professional societies to which he belongs are: Phi Eta Sigma (1944), Tau Beta Pi (1949), Sigma Xi (1951; member, 1954), and the American Physical Society (1952).

His publications are:

J. A. Stratton, P. M. Morse, L. J. Chu, J.D.C. Little, F. J. Corbató, *Spheroidal Wave Functions*, John Wiley and Sons (New York) 1956.

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Appendix A

Auxiliary Functions for Two-Center Integrals

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Printed in U. S. A.

On the Computation of Auxiliary Functions for Two-Center Integrals by Means of a High-Speed Computer*

F. J. Corbató
Massachusetts Institute of Technology, Cambridge, Massachusetts

(Received April 22, 1955)

With the view of computing simple two-center integrals by means of a high-speed computer, programs for certain basic auxiliary functions, which are essentially the usual $A_n(y)$ and $B_n(x)$, have been prepared. Computational procedures for generating these functions are given.

All two-center integrals between Slater AO's, except the exchange integrals, can be expressed[1] in terms of integrals of the type

$$y^{\alpha+\beta+\gamma+\delta+2\epsilon+1}\int_1^\infty d\xi \int_{-1}^1 d\eta e^{-y\xi-x\eta}(\xi+\eta)^\alpha(\xi-\eta)^\beta \times(1+\xi\eta)^\gamma(1-\xi\eta)^\delta(\xi^2-1)^\epsilon(1-\eta^2)^\epsilon, \quad (1)$$

where (ξ,η) are prolate spheroidal coordinates. The integrals, Eq. (1), can be expressed in terms of the auxiliary functions

$$C_n(y)=y^{n+1}e^y\int_1^\infty t^ne^{-ty}dt, \quad (y>0)$$

$$=n!\sum_{l=0}^n y^l/l!, \qquad \text{(all } y) \quad (2)$$

and

$$B_n(x)=\int_{-1}^1 t^ne^{-tx}dt=x^{-n-1}[e^xC_n(-x)-e^{-x}C_n(x)]. \quad (3)$$

The functions $C_n(y)$ are preferable to the more familiar functions,[2] $A_n(y)=y^{-n-1}e^{-y}C_n(y)$, since they permit reducing the internuclear distance to zero without numerical difficulties. Their computation presents no problem since they contain only positive terms, and if one needs the set $n=0(1)N$, the upward recursion relation

$$C_n(y)=y^n+nC_{n-1}(y) \quad (4)$$

is most convenient.

The traditional way of computing the $B_n(x)$, which corresponds to Eq. (3) has the disadvantage of rapidly losing significant figures unless x is large compared to n. To avoid this drawback a reformulation has been made using the expansion of t^n in Legendre polynomials[3] and the integral representation of the spherical hyperbolic Bessel functions of the first kind, i.e.,

$$t^n=\sum_{j=0,1}^{n}{}' a_{nj}P_j(t)$$

with

$$a_{nj}=n!(2j+1)[(n-j)!!(n+j+1)!!]^{-1}$$
$$\textstyle\sum'=\text{sum over: } j \text{ even if } n \text{ even; } j \text{ odd if } n \text{ odd} \quad (5)$$
$$n!!=n(n-2)(n-4)\cdots(2 \text{ or } 1)$$

and

$$i_n(x)=(\pi/2x)^{\frac{1}{2}}I_{n+\frac{1}{2}}(x)=\tfrac{1}{2}(-1)^n\int_{-1}^1 P_n(t)e^{-tx}dt \quad (6)$$

where $I_{n+\frac{1}{2}}(x)$ is the ordinary modified Bessel function.[4]

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* This work was assisted in part by the Office of Naval Research under Contract N5 ori 60.

[1] Ruedenberg, Roothaan, and Jaunzemis, "Laboratory of Molecular Structure and Spectra," University of Chicago, Technical Report 1952–1953, Part 2, p. 137. (To be published as a paper in this journal.) In the case considered here α, β, γ, δ, ϵ are positive exponents.

[2] E.g., see Kotani, Amemiya, and Simose, Proc. Phys.-Math. Soc. Japan **20**, Extra No. 1 (1938); Extra No. 2 (1940).

[3] E. T. Whitaker and G. N. Watson, *Modern Analysis* (Cambridge University Press, London, 1946), p. 310.

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Substitution of Eq. (5) and Eq. (6) in Eq. (3) yields

$$B_n(x)=2(-1)^n \sideset{}{'}\sum_{j=0,1}^{n} a_{nj}i_j(x). \tag{7}$$

Because the sign of $i_n(x)$ is always the same as that of x^n, it follows that the $B_n(x)$ are expressed as a sum of either all positive or all negative terms, and hence can be computed accurately by the use of Eq. (7) if the $i_n(x)$ are known.

The $i_n(x)$ are efficiently obtained by the following technique. First a set of ratios

$$r_n(x)=i_{n+1}(x)/i_n(x) \tag{8}$$

are computed using the recursion relation

$$r_{n-1}(x)=x[2n+1+xr_n(x)]^{-1} \tag{9}$$

in the numerically accurate downward direction starting from $n=M$ where r_M is made zero.[5] It can be shown that the choice[6] of $M\geqslant N+5+10|x|(N+\frac{1}{2})^{-1}$ gives seven significant figure accuracy in the ratios for $n\leqslant N$. Having obtained the ratios, the function $i_0(x)$ is found by using a relation resulting from the Wronskian of the spherical hyperbolic Bessel functions, i.e.,

$$x^2[i_n(x)k_{n+1}(x)+i_{n+1}(x)k_n(x)]=1, \tag{10}$$

where

$$k_n(x)=(2/\pi x)^{\frac{1}{2}}K_{n+\frac{1}{2}}(x).$$

For $n=0$, Eq. (10) becomes after inserting the explicit forms of $k_0(x)$ and $k_1(x)$

$$i_0(x)=e^{|x|}[1+|x|+xr_0(x)]^{-1}, \tag{11}$$

where the absolute value signs maintain a numerically-accurate form. Hence using Eq. (11) to compute $i_0(x)$, all $i_n(x)$ up to $i_N(x)$ can be computed by successive application of Eq. (8). A variation of the above procedure which avoids the cumulative round-off error of the successive ratio multiplications is the following. One puts formally

$$i_n(x)=s_n(x)i_M(x), \quad (n\leqslant M) \tag{12}$$

and determines the $s_n(x)$ by the recursion relation

$$s_{n-1}(x)=(2n+1)x^{-1}s_n(x)+s_{n+1}(x), \tag{13}$$

starting with $s_M(x)=1$, $s_{M+1}(x)=0$. Then $i_0(x)$ is found from Eq. (11), and thereby $i_M(x)$ is determined. The final step consists of the independent normalization of each $i_n(x)$ according to Eq. (12). The alternative procedure is not appropriate on a computer for very small x, because of the excessive variation of the orders of magnitude, and $x\sim 0$ must be handled as a special case of the program. It should be noted that the above procedures for determining the $i_n(x)$ are more efficient than the usual method where $i_{N-1}(x)$ and $i_N(x)$ are determined from the power series form and then used to start the downward recursion relation.

A completely automatic generation subroutine program which computes the $C_n(y)$ and $B_n(x)$ functions by the above schemes has been written for the Whirlwind computer at M.I.T., and the results indicate six to seven significant figure accuracy, a limitation due only to the computer arithmetic. For $N=6$, the time required for the computation of the $C_n(y)$ and the $B_n(x)$, $n=0(1)N$, is about a second. In addition, by using this basic subroutine, programs have been prepared for all the one-electron integrals between the orbitals 1*s*, 2*s*, and 2*p*. Each of these integrals requires between one and two seconds.

After the completion of this work, it has been brought to the author's attention that C. C. J. Roothaan has recently investigated the functions $B_n(x)$ along similar lines.

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[5] The procedure of using ratios is essentially due to J. C. P. Miller, *British Association for the Advancement of Science, Mathematical Tables*, Vol. X, *Bessel Functions*, Part II (University Press, Cambridge, 1952), p. xvi.

[6] A better but more elaborate expression for M can also be found—in any case, unduly high values of M are avoided by using the closed form, or, equivalently, the *upward* recursion formula for the $i_n(x)$ when $x>4N+2$.

Appendix B

Secular Equation Utility Programs

Memorandum DCL-58 Page 1 of 12 pages

Digital Computer Laboratory
Massachusetts Institute of Technology
Cambridge 39, Massachusetts

SUBJECT: PROGRAMS FOR SOLVING SECULAR EQUATIONS

To: Scientific and Engineering Computation Group

From: F.J. Corbató

Introduction

Production programs for Whirlwind I are now available for solving two types of secular equations by use of the techniques described in a report by A. Meckler[1] and are summarized briefly below. These are the ordinary variety, (case I), $\sum_j H_{ij}\psi_{jk} = \psi_{ik}\lambda_k$, and the general variety, (case II), $\sum_j H_{ij}\psi_{jk} = \sum_j S_{ij}\psi_{jk}\lambda_k$, where $k = 1, 2, \ldots, n$, H and S are real symmetric matrices and S is positive definite. The two programs, for case I and for case II, can handle matrices of order $1 \leq n \leq 32$. The results are given photographically and consist of the input data and the λ_k and ψ_{jk} where in case I, $\sum_j \psi_{ij}^{\dagger}\psi_{jk} = \delta_{ik}$ and in case II, $\sum_{i,j} \psi_{\ell i}^{\dagger} S_{ij}\psi_{jk} = \delta_{\ell k}$. In addition the intermediate results of case II, if desired may be displayed.

Methods of Solution

Matrix diagonalization is the elementary process used to solve both cases. The diagonalization of a symmetric matrix $M_{\ell k} = M_{k\ell}$ is accomplished by successive 2 by 2 "rotations" of all the matrix elements associated with the indices i and j where M_{ij} is the largest off-diagonal element. It can be simply shown that such a process converges. The explicit transformations applied are:

---

[1] A. Meckler, Quarterly Progress Report, Solid-State and Molecular Theory Group, M.I.T., Oct. 15, 1954, p. 15.

$$
\begin{aligned}
M'_{\ell k} &= M_{\ell k} & \ell \neq i,j \quad & k \neq i,j \\
M'_{ik} &= cM_{ik} + sM_{jk} & & k \neq i,j \\
M'_{jk} &= -sM_{ik} + cM_{jk} & & k \neq i,j \\
M'_{ii} &= c^2M_{ii} + 2scM_{ij} + s^2M_{jj} & & \\
M'_{jj} &= s^2M_{ii} - 2scM_{ij} + c^2M_{jj} & & \\
M'_{ij} &= 0 & &
\end{aligned}
$$

where

$$c = \sqrt{\frac{1}{1 + t^2}}$$

$$s = tc$$

and

$$
t = \begin{cases}
\dfrac{(M_{ii} - M_{jj}) + \sqrt{(M_{ii} - M_{jj})^2 + 4(M_{ij})^2}}{-2M_{ij}} , & (M_{ii} > M_{jj}) \\[2ex]
\dfrac{+2M_{ij}}{(M_{ii} - M_{jj}) - \sqrt{(M_{ii} - M_{jj})^2 + 4(M_{ij})^2}} , & (M_{ii} \leqslant M_{ij})
\end{cases}
$$

Similarly, the unitary transformation, U , (initially a diagonal unit matrix), is modified after each 2 by 2 rotation by the corresponding transformation affecting the <u>ith</u> and <u>jth</u> columns.

$$
\begin{aligned}
U'_{km} &= U_{km} & m \neq i,j \\
U'_{ki} &= cU_{ki} + sU_{kj} & \\
U'_{kj} &= -sU_{ki} + cU_{kj} &
\end{aligned}
$$

This process continues until $M_{ij} < 2^c$, where c is the preset criterion value, the result being that the diagonal of the final M_{ij} (i.e. the eigenvalues, λ) and the final U satisfy the conditions:

$$\sum_{j=1}^{n} M_{ij}U_{jk} = U_{ik}\lambda_k \quad \text{or} \quad MU = U\lambda$$

(where λ does not multiply as a vector but as a scalar)

In nearly all applications, the original matrix, M, was computed from an operator, $\mathfrak{m}$, by means of a set of basis states. These states can be represented as a set of unit vectors, $\vec{e}_i$, in a Hilbert space, and what is desired is the transformation which when applied to the original basis states gives a new set of basis states that when applied to the operator $\mathfrak{m}$, yield a diagonal matrix. To obtain this transformation it is noted that if

$$M_{ij} = \langle \vec{e}_i | \mathfrak{m} | \vec{e}_j \rangle$$

and

$$\delta_{\ell k} \lambda_k = \sum_{i,j} U^{\dagger}_{\ell i} M_{ij} U_{jk}$$

then

$$\delta_{\ell k} \lambda_k = \sum_{i,j} U^{\dagger}_{\ell i} \langle \vec{e}_i | \mathfrak{m} | \vec{e}_j \rangle U_{jk}$$

$$= \left\langle \sum_i U^{\dagger}_{\ell i} \vec{e}_i \middle| \mathfrak{m} \middle| \sum_j U^{\dagger}_{kj} \vec{e}_j \right\rangle$$

$$= \langle \vec{e}\,'_{\ell} | \mathfrak{m} | \vec{e}\,'_k \rangle$$

Thus the desired transformation is $\vec{e}\,'_k = \sum_j U^{\dagger}_{kj} \vec{e}_j$. Stated in another manner, the k<u>th</u> eigenvalue of M is associated with an eigenvector consisting of the k<u>th</u> column-vector of U_{jk} where the components of the eigenvector refer to the original basis states used to compute M.

For case II, the procedure of solution is the following. First S is diagonalized so that $SU_{S'} = U_{S'}S'$, where S' is diagonal. Then $S^{-1/2}$ is formed where $S^{-1/2} = U_{S'}(S')^{-1/2}U^{\dagger}_{S'}$, and the new matrix H' is formed by matrix multiplication where $H' = S^{-1/2}HS^{-1/2}$. Then a second diagonalization is made such that

$$H' U_{H'} = U_{H'} \lambda \quad .$$

and finally $\Psi = S^{-1/2}U_{H'}$, where it is seen that $\Psi^{\dagger} S \Psi = 1$.

To verify that this λ and Ψ form desired solutions, it is observed that

$$H\psi = HS^{-1/2}U_{H'} = \left[U_{S'}(S')^{1/2}U_{S'}^{\dagger}U_{S'}(S')^{-1/2}U_{S'}^{\dagger}\right] HS^{-1/2}U_{H'} =$$

$$= S^{1/2}H'U_{H'} = S^{1/2}U_{H'}\lambda =$$

$$= \left[U_{S'}(S')^{1/2}U_{S'}^{\dagger}\right]\left[U_{S'}(S')^{1/2}U_{S'}^{\dagger}U_{S'}(S')^{-1/2}U_{S'}^{\dagger}\right] U_{H'}\lambda$$

$$= SS^{-1/2}U_{H'}\lambda$$

$$= S\psi\lambda \quad .$$

Specification of Input Data

Both programs have their input data, (also called parameter sets), located in the same storage locations and moreover do not destroy during operation any of the necessary input information. Thus a series of secular equations each differing from the previous by the addition of a row and column could be conveniently solved by supplying the complete matrix (or pair of matrices in case II) in the first parameter tape and then merely changing the matrix order, n, for each subsequent parameter. Furthermore, a parameter tape for case II could be used with program I, but would, of course, give solutions for case I. (Program I would also disturb the storage of the unnecessary S matrix.)

In the listing of the input data, two types of number conventions are used. These are the single-register (15,0) integer, (less than 32768 in magnitude), which may have a sign but no decimal point, and the double-register (24,6) generalized decimal number which must have both a sign and a decimal point. The specific locations of the input data are:

34	$+n$	matrix order, $1 \leqslant n \leqslant 32$	(15,0) integers
35	$+c_S$	diagonalization criterion of S, $c_S \geqslant -60$	
36	$+c_H$	diagonalization criterion of H, $c_H \geqslant -60$	
37	$+k$	identification number	
2048	$+H_{11}$	listing of the H matrix	

(continued on next page)

$+H_{12}$
$+H_{22}$
$+H_{13}$
$+H_{23}$
。。。。
$+H_{nn}$ (24,6)
3104| $+S_{11}$ listing of the S matrix numbers
$+S_{12}$
$+S_{22}$
$+S_{13}$
$+S_{23}$
。。。。
$+S_{nn}$

Both programs start at register 32 decimal and stop on an "si 0" instruction in register 33 decimal (41 octal)。 If many sets of parameters are to be included in one big tape and are to be automatically run consecutively, all but the last set should contain an additional 33| sp26, and the last set should contain a 33| si0。 Each set on a multiple-parameter tape must be preceded by a "fc" and then a "(24,6)"; the performance request should have, under the heading of operation instructions, a "Turn off si 1 switch" on the line preceding the multiple-parameter tape operation instruction。

Criterion Values

The values of C_H and C_S are used to terminate the diagonalization procedures after sufficient accuracy has been obtained。 For both the H and the S diagonalization, each c should be chosen such that

$$\frac{2^c}{|\lambda_i - \lambda_j|_{\max}} \lesssim \frac{\left|\underline{\text{maximum absolute error in eigenvector components}}\right|}{1} \simeq \frac{\left|\underline{\text{maximum absolute error in eigenvalues}}\right|}{|\lambda_k|_{\max}}$$

The accuracy of the computations is such that the right-hand side of the above relation can never be made less than about 10^{-7}. Empirical values for this last figure are:

	Case I ($n = 5$)	Case II ($n = 5$)
Eigenvalues:	1×10^{-7}	4×10^{-7}
Eigenvectors:	2×10^{-7}	5×10^{-7}

	Case I ($n = 18$)
Eigenvalues:	3×10^{-7}
Eigenvectors:	8×10^{-7}

For an example of the determination of c, suppose that 6 figures were designed in the eigenvectors and that $|\lambda_i - \lambda_j|_{max} \sim 3$. Then

$$2^c \leq 3 \times \frac{\frac{1}{2} \times 10^{-7}}{1} = 150 \times 10^{-9} < 256 \times 10^{-9} \cong 2^8 2^{-30} = 2^{-24}$$

and therefore $c_{max} \cong -24$. (A useful relation is that $2^{10} = 1024 \cong 10^{+3}$). In practice, one would probably use $+c = -30$ to be certain of the desired accuracy. As is implied, the value of c can always be safely lowered (except not below approximately -60) since the only effect will be to raise the computation time somewhat (i.e. at worst up to 50 or 100% more time). For case II when the eigenvalues of S and H are both of the same order, c_S and c_H should be about the same, since the overall accuracy is determined by the least accurate diagonalization.

Form of Output

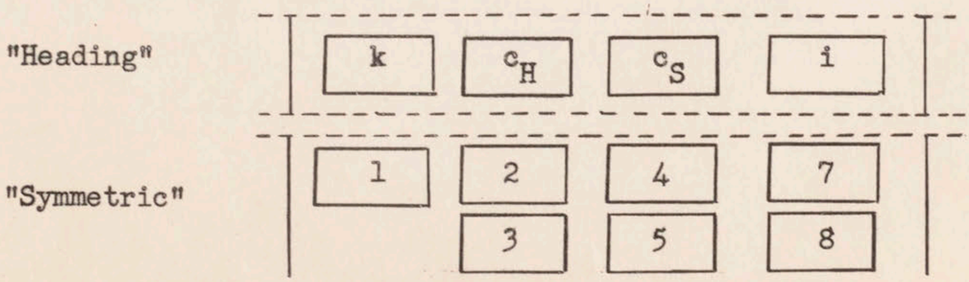
All of the program output is given photographically with each secular equation solution beginning on a new frame. The various displays may be divided into three classes: 1) the initial data, 2) the intermediate results (case II only), and 3) the final results. Each display of the first two classes will consist of a "heading" line followed by either a "symmetric" or "square" pattern of the pertinent numbers. The third class consists of a heading line followed by the "rectangular" pattern of λ_k in the first column and then the Ψ_{j1} to Ψ_{jn}, each in a column, starting from the third column. The first class is normally displayed but may be suppressed, the second class is normally suppressed but may be displayed, and the third class is always displayed. The program will use as many frames as are necessary to include all the displays, starting on a new frame if a particular display will not entirely fit on the remainder of a frame.

The "heading" line will have in the first column, the identifying code number of the solution, k; in the second column the criterion value, c_H (except on the display of S); in the third column the criterion value c_S, (except on the display of H); and in the fourth column, an intermediate result identification number, i, (only for class 2 displays). Case I results may be distinguished from Case II results by the absence of c_S in the result heading line.

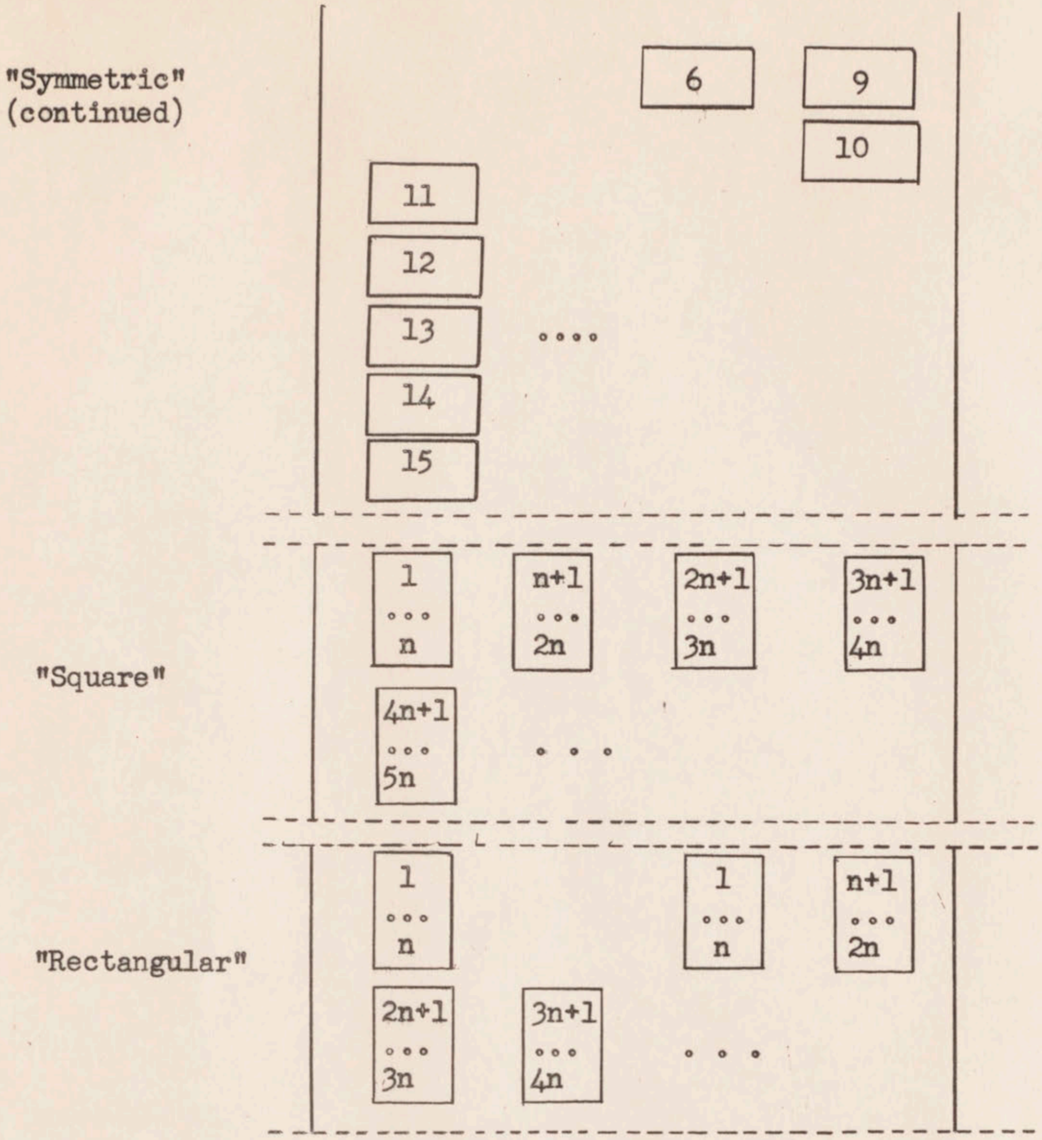
The selection or suppression of the various displays depends on the contents of the associated suppressor registers: +0 for display; -0 for suppression. These displays and their suppressor registers are:

	Display	Contents	Pattern	Decimal Address of Suppressor Register
Class 1	H	H	sym.	1598
	S	S	sym.	
Class 2	1	S'	sym.	1599
	2	$U_{S'}$	sq.	1600
	3	$S^{-1/2}$	sym.	1601
	4	$HS^{-1/2}$	sq.	1602
	5	H'	sym.	1603
	6	$U_{H'}$	sq.	1604
Class 3	$\lambda + \psi$	$\lambda + \psi$	rect.	——

Symbolically, we have for the various forms of output:



(continued on next page)



The total number of film frames required per solution depends on the number of displays not suppressed but may be computed from the schedules given below. If two or more displays are to fit on the same frame, they will be separated by two additional spacing lines beyond that given in the schedules. (For $n > 8$, no two displays will fit on the same frame.) Each frame can contain a maximum of 36 lines.

	number of lines (or frames = f)		
matrix order	head. + sym.	head. + sq.	head. + rect.
1	3	3	3
2	4	4	4
3	5	5	9

(continued on next page)

4	6	6	11
5	12	13	13
6	13	15	15
7	14	17	25
8	15	19	28
9-10	f	f	f
11-12	f	2f	2f
13-14	2f	2f	2f
15-16	2f	2f	3f
17	2f	3f	3f
18	2f	5f	5f
19	2f	5f	6f
20	3f	5f	6f
21-22	4f	6f	6f
23-24	4f	6f	7f
25-26	5f	7f	7f
27-28	5f	7f	8f
29-30	6f	8f	8f
31-32	6f	8f	9f

For convenience the most common situations are summarized:

	number of frames per solution		
matrix order	normal case I	normal case II	full suppression of cases I and II
1-4	1	1	1
5-6	1	2	1
7-8	2	2	1
9-10	2	3	1
11-12	3	4	2
13-14	4	6	2
15-17	5	7	3
18	7	9	5
19	8	10	6
20	9	12	6

(continued on next page)

21-22	10	14	6
23-24	11	15	7
25-26	12	17	7
27-28	13	18	8
29-30	14	20	8
31-32	15	21	9

Information for Filling Out Performance Requests

1. Time estimates: These are difficult to state in general but roughly $T_{\text{case II}} \cong 2T_{\text{case I}}$ and $T_{\text{case I}} \cong Kn^3$ where $K \sim \frac{1}{10}$ sec. Variations from this formula depend on the difficulty of diagonalization (i.e. on the size of the off-diagonal elements and the stringency of the criteria). *

2. Program stop: Stops automatically on si0 in register 41 octal.

3. Camera output: See film frame schedules above for the number of frames per solution. Camera first used in 0 sec.

4. Magnetic drum: Case I uses auxiliary drum groups 1, 2, 3; case II uses auxiliary drum groups 1, 2, 3, 4. Drum first used in 0 sec.

5. Operating instructions: These are for a single-parameter tape

E, fb A , RI,
fb 10172-20-B, RI,
fc C , RI, RS.

where A = "dummy logging tape"; (tape room will prepare this)

$$B = \begin{cases} 334, \text{ (case I)} \\ 331, \text{ (case II)} \end{cases}$$

C = parameter tape number

For multiple-parameter tapes, the corresponding instructions are

E, fb A , RI,
fb ~~1072~~ 10172-20-B, RI,
Turn off si 1 switch
fc C , RI.

---

* An additional time of about 10 seconds must be added for each full frame displayed.

Program Alarms

	Type of Alarm	Octal Identification	Immediate Cause	Probable Cause
1.	Check register	PC = 3764 AR = 3453	GD no. unscale-factored	a
2.	Check register	PC = 3764 AR = 3503	GD no. in MRA too large to store	a,b
3.	Check register (case II only)	PC = 2601	An eigenvalue of S is <0	a,b,c
4.	Divide error (case II only)	PC = 3612	An eigenvalue of S = 0	a,b,c

Probable Causes

a. GD number of initial data out of phase, due to either a missing decimal point, a missing seventh hole in the tape, an incorrect storage address, or a faulty parameter tape read-in by the computer. Compare print of data tape with display of input data.

b. Input data is very poorly scale-factored or, (case II only), one of the eigenvalues of S is extremely small.

c. The matrix S is not positive definite.

Additional Remarks for Experienced Programmers

1. If matrix elements are to be generated, decimal registers 38 to 1563 inclusive are available for programs and will be restored after each solution. Additional storage is available on the auxiliary drum starting at the decimal address 7630 (case I) and 10206 (case II). All generation program tapes must have a NOT PA included; the PA already in the program contains buffers b and 6b inclusive and a single cycle counter. Thus all cycle instructions may be used, but no "isc" orders (except isc0). Buffers b through 3b are used as temporary storage during a solution and 4b through 6b are unused.

2. The program also contains a DIB/DOB subroutine; the decimal entries are:

<u>for DIB</u>		<u>for DOB</u>
sp1605		sp1610
[CM]	core memory address	[CM]
[DA]	aux. drum address	[DA]
w	no. of reg. to transfer	w
←	return point in wi mode	→

F. J. Corbató

F.J. Corbató
March 15, 1955

Appendix C

Integral Values

TABLE C-1

Energy band interpolation integral values obtained by Slater and Koster for the diamond crystal, (private communication). These integrals were used for the interpolation example of the graphite crystal given in figure 7-3. For λ values not listed, the integrals were set equal to zero. The integrals are listed in symmetric matrices of vectors where each vector is a list of the integrals for the $\lambda\mu\nu$ values: 000, 100, 200. Energy units are in Rydbergs.

Hamiltonian Integrals: $H_{jj'}(\lambda\mu\nu)$

j' j	1sσ	2sσ	2pσ	2pπ	2p$\bar{\pi}$
1sσ	-20. 0 0	0 0 0	0 0 0	0 0 0	0 0 0
2sσ		-1.45 -.33 +.03	0 -.25 -.03	0 0 0	0 0 0
2pσ			+.45 -.61 -.04	0 0 0	0 0 0
2pπ				+.45 +.22 +.05	0 0 0
2p$\bar{\pi}$					-.45 -.22 -.05

TABLE C-1 (cont.)

Overlap Integrals: $S_{jj'}(\lambda\mu\nu)$

$j \backslash j'$	1sσ	2sσ	2pσ	2pπ	2p$\bar{\pi}$
1sσ	+1. 0 0	0 0 0	0 0 0	0 0 0	0 0 0
2sσ		+1. 0 0	0 0 0	0 0 0	0 0 0
2pσ			-1. 0 0	0 0 0	0 0 0
2pπ				-1. 0 0	0 0 0
2p$\bar{\pi}$					+1. 0 0

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TABLE C-2

Overlap and kinetic energy integrals used for figure 7-1 solution. These integrals, which only depend on λ , are listed in symmetric matrices of vectors where each vector represents the integrals for the λ values: 0, 1, 2, 3, 4, 5, 6, 7, 8, 9. Non-significant zeros are omitted for legibility. Energy units are two Rydbergs.

Overlap Integrals: $S_{jj'}(\lambda\mu\nu)$

$j \backslash j'$	$1s\sigma$	$2s\sigma$	$2p\sigma$	$2p\pi$	$2p\bar{\pi}$
$1s\sigma$	+1.00000	+.00006	+.00000	+.00000	+.00000
	+. 9	-. 4407	+. 8308	0	0
	0	-. 446	+. 1365	0	0
	0	-. 186	+. 697	0	0
	0	-. 21	+. 133	0	0
	0	-. 6	+. 53	0	0
	0	-. 1	+. 15	0	0
	0	-. 1	+. 10	0	0
	0	0	+. 4	0	0
	0	0	+. 1	0	0
$2s\sigma$		+1.00000	-.00000	+.00000	+.00000
		+.40955	-.45082	0	0
		+. 9923	-.16985	0	0
		+. 5383	-.10580	0	0
		+. 1080	-. 2939	0	0
		+. 420	-. 1369	0	0
		+. 116	-. 479	0	0
		+. 77	-. 345	0	0
		+. 25	-. 135	0	0
		+. 8	-. 56	0	0

TABLE C-2 (cont.)

Overlap Integrals (cont.): $S_{jj'}(\lambda\mu\nu)$

$j \backslash j'$	$1s\sigma$	$2s\sigma$	$2p\sigma$	$2p\pi$	$2p\bar{\pi}$
$2p\sigma$			-1.00000	+.00000	+.00000
			+.24397	0	0
			+.19386	0	0
			+.14020	0	0
			+. 5238	0	0
			+. 2812	0	0
			+. 1170	0	0
			+. 886	0	0
			+. 398	0	0
			+. 187	0	0
$2p\pi$				-1.00000	+.00000
				-.31310	0
				-. 7600	0
				-. 4351	0
				-. 1070	0
				-. 481	0
				-. 165	0
				-. 118	0
				-. 46	0
				-. 19	0
$2p\bar{\pi}$					+1.00000
					+.31310
					+. 7600
					+. 4351
					+. 1070
					+. 481
					+. 165
					+. 118
					+. 46
					+. 19

TABLE C-2 (cont.)

Kinetic Energy Integrals: $T_{\alpha\alpha'}(\lambda\mu\nu)$

$\alpha \backslash \alpha'$	1sσ	2sσ	2pσ	2pπ	2p$\bar{\pi}$
1sσ	+16.06086	+4.17349	+.00000	+.00000	+.00000
	-. 49	+. 805	+. 707	0	0
	0	+. 198	-. 244	0	0
	0	+. 94	-. 156	0	0
	0	+. 13	-. 41	0	0
	0	+. 4	-. 18	0	0
	0	+. 1	-. 6	0	0
	0	+. 1	-. 4	0	0
	0	0	-. 1	0	0
	0	0	-. 1	0	0
2sσ		+1.54411	-.00000	+.00000	+.00000
		+. 5475	-.15845	0	0
		-. 1201	-. 529	0	0
		-. 1006	+. 392	0	0
		-. 337	+. 455	0	0
		-. 154	+. 277	0	0
		-. 50	+. 121	0	0
		-. 34	+. 92	0	0
		-. 12	+. 40	0	0
		-. 4	+. 18	0	0

TABLE C-2 (cont.)

Kinetic Energy Integrals (cont.): $T_{ii'}(\lambda\mu\nu)$

i \ i'	1sσ	2sσ	2pσ	2pπ	2p$\bar{\pi}$
2pσ			-1.24920	+.00000	+.00000
			+.24684	0	0
			+. 4117	0	0
			+. 1602	0	0
			-. 169	0	0
			-. 243	0	0
			-. 167	0	0
			-. 139	0	0
			-. 77	0	0
			-. 41	0	0
2pπ				-1.24920	+.00000
				-. 9850	0
				-. 411	0
				+. 7	0
				+. 107	0
				+. 67	0
				+. 30	0
				+. 23	0
				+. 10	0
				+. 5	0
2p$\bar{\pi}$					+1.24920
					+. 9850
					+. 411
					-. 7
					-. 107
					-. 67
					-. 30
					-. 23
					-. 10
					-. 5

TABLE C-3

Two-center potential integrals obtained by the procedures of chapter 4. These integrals, which depend only on λ, are listed in symmetric matrices of vectors where each vector represents the integral value for the necessary λ =0, 1, 2, 3, 4, 5, 6, 7, 8, 9. Non-significant zeros are omitted for legibility. Energy units are two Rydbergs.

Potential Integrals: $\frac{1}{3}\sum_{\nu'=0}^{2} P_{ii'}(000|\lambda'\mu'\nu')$

$i \backslash i'$	1sσ	2sσ	2pσ	2pπ	2p$\bar{\pi}$
1sσ	+23.82009	+3.84874	+.00000	+.00000	+.00000
	+. 2964	-. 128	0	0	0
	+. 52	-. 2	0	0	0
	+. 12	-. 1	0	0	0
	0	0	0	0	0
	0	0	0	0	0
	0	0	0	0	0
	0	0	0	0	0
	0	0	0	0	0
	0	0	0	0	0
2sσ		+1.51502	+.00000	+.00000	+.00000
		+. 8397	0	0	0
		+. 272	0	0	0
		+. 72	0	0	0
		+. 3	0	0	0
		0	0	0	0
		0	0	0	0
		0	0	0	0
		0	0	0	0
		0	0	0	0

TABLE C-3 (contd.)

Potential Integrals (contd.): $\frac{1}{3}\sum_{\nu'=0}^{2} P_{jj'}(000|\lambda'\mu'\nu')$

j \ j'	1sσ	2sσ	2pσ	2pπ	2p$\bar{\pi}$
2pσ			-.96436	+.00000	+.00000
			-.11216	0	0
			-. 552	0	0
			-. 171	0	0
			-. 9	0	0
			-. 2	0	0
			0	0	0
			0	0	0
			0	0	0
			0	0	0
2pπ				-.96436	+.00000
				-.11216	0
				-. 552	0
				-. 171	0
				-. 9	0
				-. 2	0
				0	0
				0	0
				0	0
				0	0
2p$\bar{\pi}$					+.96436
					+. 3328
					+. 112
					+. 31
					+. 1
					0
					0
					0
					0
					0

TABLE C-3 (contd.)

Potential Integrals : $P_{ii'}(\lambda\mu\nu|000)$

$i \backslash i'$	1sσ	2sσ	2pσ	2pπ	2p$\bar{\pi}$
1sσ	+23.82009	+3.84874	+.00000	+.00000	+.00000
	+. 23	-.38821	+.75232	0	0
	0	-. 3815	+.12021	0	0
	0	-. 1583	+. 6113	0	0
	0	-. 179	+. 1160	0	0
	0	-. 53	+. 457	0	0
	0	-. 10	+. 132	0	0
	0	-. 6	+. 90	0	0
	0	-. 2	+. 31	0	0
	0	0	+. 12	0	0
2sσ		+1.51502	-.00000	+.00000	+.00000
		+.11411	-.18611	0	0
		+. 1362	-. 3634	0	0
		+. 588	-. 1905	0	0
		+. 72	-. 382	0	0
		+. 22	-. 154	0	0
		+. 4	-. 46	0	0
		+. 3	-. 31	0	0
		+. 1	-. 11	0	0
		0	-. 4	0	0

TABLE C-3 (contd.)

Potential Integrals (contd.): $P_{ii'}(\lambda\mu\nu|000)$

i \ i'	1sσ	2sσ	2pσ	2pπ	2p$\bar{\bar{\pi}}$
2pσ			-.96436	+.00000	+.00000
			+.15470	0	0
			+. 3054	0	0
			+. 1607	0	0
			+. 327	0	0
			+. 133	0	0
			+. 40	0	0
			+. 27	0	0
			+. 10	0	0
			+. 4	0	0
2pπ				-.96436	+.00000
				-. 7022	0
				-. 724	0
				-. 324	0
				-. 48	0
				-. 17	0
				-. 4	0
				-. 3	0
				-. 1	0
				0	0
2p$\bar{\bar{\pi}}$					+.96436
					+. 7022
					+. 724
					+. 324
					+. 48
					+. 17
					+. 4
					+. 3
					+. 1
					0

TABLE C-3 (contd.)

Potential Integrals: $P_{\alpha\alpha}'(\lambda\mu\nu|\lambda\mu\nu)$

$\alpha \backslash \alpha'$	1sσ	2sσ	2pσ	2pπ	2p$\bar{\pi}$
1sσ	+23.82009	+3.84874	+.00000	+.00000	+.00000
	+. 23	-. 235	+. 406	0	0
	0	-. 1	+. 1	0	0
	0	0	0	0	0
	0	0	0	0	0
	0	0	0	0	0
	0	0	0	0	0
	0	0	0	0	0
	0	0	0	0	0
	0	0	0	0	0
2sσ		+1.51502	-.00000	+.00000	+.00000
		+.11411	-.11150	0	0
		+. 1362	-. 1382	0	0
		+. 588	-. 603	0	0
		+. 72	-. 75	0	0
		+. 22	-. 23	0	0
		+. 4	-. 5	0	0
		+. 3	-. 3	0	0
		+. 1	-. 1	0	0
		0	0	0	0

TABLE C-3 (contd.)

Potential Integrals (contd.): $P_{ii'}(\lambda\mu\nu|\lambda\mu\nu)$

$i \backslash i'$	$1s\sigma$	$2s\sigma$	$2p\sigma$	$2p\pi$	$2p\bar{\pi}$
$2p\sigma$			-.96436	+.00000	+.00000
			+.15470	0	0
			+. 3054	0	0
			+. 1607	0	0
			+. 327	0	0
			+. 133	0	0
			+. 40	0	0
			+. 27	0	0
			+. 10	0	0
			+. 4	0	0
$2p\pi$				-.96436	+.00000
				-. 7022	0
				-. 724	0
				-. 324	0
				-. 48	0
				-. 17	0
				-. 4	0
				-. 3	0
				-. 1	0
				0	0
$2p\bar{\pi}$					+.96436
					+. 7022
					+. 724
					+. 324
					+. 48
					+. 17
					+. 4
					+. 3
					+. 1
					0

TABLE C-4

Hamiltonian integrals computed from two-center integrals of tables C-2 and C-3. These integrals, which were used (along with the overlap integrals of table C-2) for the solution of fig. 7-5, depend only on λ and are listed in a symmetric matrix of vectors where each vector represents the integrals for the values λ = 0, 1, 2, 3, 4, 5, 6, 7, 8, 9. Non-significant zeros are omitted for legibility. Energy units are two Rydbergs.

Hamiltonian Integrals: $H_{ii'}(\lambda\mu\nu)$

$i \backslash i'$	1sσ	2sσ	2pσ	2pπ	2p$\bar{\pi}$
1sσ	-7.85167	+.32874	-.00000	+.00000	+.00000
	-. 94	+.39861	-.74932	0	0
	0	+. 4014	-.12267	0	0
	0	+. 1678	-. 6269	0	0
	0	+. 192	-. 1201	0	0
	0	+. 57	-. 475	0	0
	0	+. 11	-. 138	0	0
	0	+. 7	-. 94	0	0
	0	+. 2	-. 32	0	0
	0	0	-. 12	0	0
2sσ		-.24154	+.00000	+.00000	+.00000
		-.17347	+.13916	0	0
		-. 3924	+. 4488	0	0
		-. 2182	+. 2900	0	0
		-. 480	+. 911	0	0
		-. 197	+. 453	0	0
		-. 58	+. 171	0	0
		-. 40	+. 126	0	0
		-. 13	+. 52	0	0
		-. 5	+. 23	0	0

TABLE C-4 (cont.)

Hamiltonian Integrals (cont.): $H_{jj'}(\lambda\mu\nu)$

$j \backslash j'$	$1s\sigma'$	$2s\sigma'$	$2p\sigma'$	$2p\pi'$	$2p\bar{\pi}'$
$2p\sigma$			+.09060	+.00000	+.00000
			-. 6257	0	0
			-. 1992	0	0
			-. 1613	0	0
			-. 823	0	0
			-. 508	0	0
			-. 246	0	0
			-. 194	0	0
			-. 96	0	0
			-. 49	0	0
$2p\pi$				+.09060	+.00000
				+. 4195	0
				+. 1036	0
				+. 656	0
				+. 203	0
				+. 101	0
				+. 39	0
				+. 29	0
				+. 12	0
				+. 5	0
$2p\bar{\pi}$					+.17724
					-. 4195
					-. 1036
					-. 656
					-. 203
					-. 101
					-. 39
					-. 29
					-. 12
					-. 5

TABLE C-5

Two- and three-center potential integrals computed by the techniques of chapter 5. Parentheses indicate corrections based on the two-center integrals of table C-3. It is noted that

$$V_{jj'}(\lambda\mu\nu) = \sum_{\lambda'\mu'\nu'} P_{jj'}(\lambda\mu\nu|\lambda'\mu'\nu')$$

where the $V_{jj'}$ values listed include the parenthetical corrections. Energy units are 2×10^{-5} Rydbergs. The P integrals given are rounded off from the precise values used in the computer to obtain the V integrals.

Potential Integrals: $P_{jj'}(000|\lambda'\mu'\nu')$

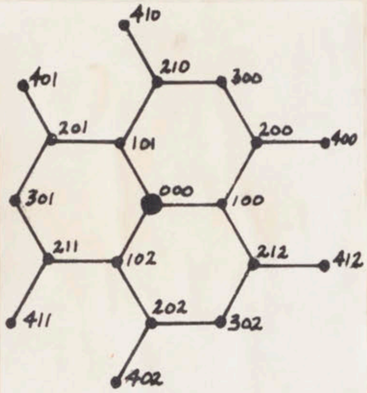

FIG. C-1

$\lambda'\mu'\nu'$ j, j'=	$1s\sigma,1s\sigma$	$1s\sigma,2s\sigma$	$1s\sigma,2p\sigma$	$1s\sigma,2p\pi$	$2s\sigma,2s\sigma$	$2s\sigma,2p\sigma$
000	+2382028	+384879	0	0	+151503	0
100	+3037	-232	-565	0	+8352	+11740
101	+3037	-232	+283	+489	+8352	-5870
102	+3037	-232	+283	-489	+8352	-5870
200	+76	-5	-8	+5	+271	+414
210	+76	-5	0	+9	+271	0
201	+76	-5	+8	+5	+271	-414
211	+76	-5	+8	-5	+271	-414
202	+76	-5	0	-9	+271	0
212	+76	-5	-8	-5	+271	+414
300	+21	-1	-1	+2	+72	+68
301	+21	-1	+2	0	+72	-136
302	+21	-1	-1	-2	+72	+68
400	+1	0	0	0	+3	+6
410	+1	0	0	0	+3	-1
401	+1	0	0	0	+3	-5
411	+1	0	0	0	+3	-5
402	+1	0	0	0	+3	-1
412	+1	0	0	0	+3	+6
(higher neighbors)	(+1)	(0)	(0)	(0)	(+3)	(0)
$V_{jj'}(000)$	+2391665	+384148	0	0	+178417	0

TABLE C-5 (contd.)

Potential Integrals (contd.): $\rho_{jj'}(000|\lambda'\mu'\nu')$

$\lambda'\mu'\nu'$ $j, j'=$	$2s\sigma, 2p\pi$	$2p\sigma, 2p\sigma$	$2p\sigma, 2p\pi$	$2p\pi, 2p\pi$	$2p\bar{\pi}, 2p\bar{\pi}$
000	0	-96436	0	-96436	+96436
100	0	-19103	0	-3323	+3323
101	-10167	-7268	-6833	-15158	+3323
102	+10167	-7268	+6833	-15158	+3323
200	-239	-772	+382	-331	+111
210	-478	-111	0	-992	+111
201	-239	-772	-382	-331	+111
211	+239	-772	+382	-331	+111
202	+478	-111	0	-992	+111
212	+239	-772	-382	-331	+111
300	-118	-101	+121	-241	+31
301	0	-311	0	-31	+31
302	+118	-101	-121	-241	+31
400	-2	-16	+5	-3	+1
410	-6	-2	-3	-17	+1
401	-4	-10	-8	-8	+1
411	+4	-10	+8	-8	+1
402	+6	-2	+3	-17	+1
412	+2	-16	-5	-3	+1
(higher neighbors)	(0)	(-13)	(0)	(-13)	(+2)
$V_{jj'}(000)$	0	-133967	0	-133967	+107174

TABLE C-5 (contd.)

Potential Integrals: $P_{jj'}(100|\lambda'\mu'\nu')$

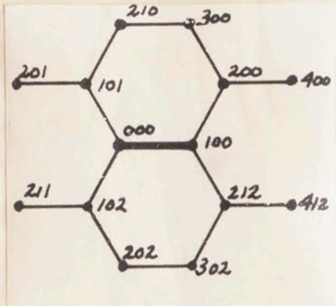

FIG. C-2

$\lambda'\mu'\nu'$	$j,j'=$ $1s\sigma,1s\sigma$	$1s\sigma,2s\sigma$	$1s\sigma,2p\sigma$	$1s\sigma,2p\pi$	$2s\sigma,2s\sigma$	$2s\sigma,2p\sigma$
000	+23	-38821	+75232	0	+11411	-18611
100	+23	-235	+406	0	+11411	-11150
200	0	-4	+7	+1	+1043	+297
101	0	-127	+249	+21	+1043	-2215
102	0	-127	+249	-21	+1043	-2215
212	0	-4	+7	-1	+1043	+297
300	0	-1	+1	0	+96	-44
210	0	-3	+5	+1	+96	-145
202	0	-3	+5	-1	+96	-145
302	0	-1	+1	0	+96	-44
400	0	0	0	0	+19	+22
201	0	-2	+4	0	+19	-60
211	0	-2	+4	0	+19	-60
412	0	0	0	0	+19	+22
$V_{jj'}(100)$	+46	-39330	+76171	0	+27456	-34049

$\lambda'\mu'\nu'$	$j,j'=$ $2s\sigma,2p\pi$	$2p\sigma,2p\sigma$	$2p\sigma,2p\pi$	$2p\pi,2p\pi$	$2p\bar{\pi},2p\bar{\pi}$
000	0	+15470	0	-7022	+7022
100	0	+15470	0	-7022	+7022
200	-1298	-1069	+2798	-1603	+255
101	-1016	-1069	-330	-1603	+255
102	+1016	-1069	+330	-1603	+255
212	+1298	-1069	-2798	-1603	+255
300	-175	+21	+273	-372	+19
210	-170	+21	+69	-372	+19
202	+170	+21	-69	-372	+19
302	+175	+21	-273	-372	+19
400	-18	-87	+59	-26	+7
201	-17	-87	-23	-26	+7
211	+17	-87	+23	-26	+7
412	+18	-87	-59	-26	+7
$V_{jj'}(100)$	0	+26401	0	-22046	+15167

TABLE C-5 (contd.)

Potential Integrals: $V_{jj'}(200|\lambda'\mu'\nu')$

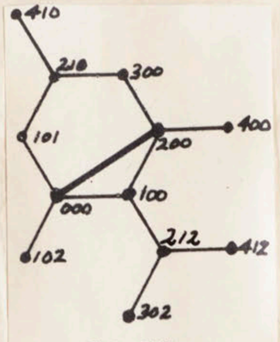

FIG. C-3

$\lambda'\mu'\nu'$ j, j'=	1sσ,1sσ	1sσ,2sσ	1sσ,2pσ	1sσ,2pπ	2sσ,2sσ	2sσ,2pσ
000	0	-3815	+12021	0	+1362	-3634
200	0	-1	+1	0	+1362	-1382
100	0	-24	+66	-4	+3452	-5958
300	0	0	0	0	+324	-164
101	0	-15	+47	+3	+324	-921
210	0	0	+1	0	+109	-176
212	0	0	+1	0	+109	-176
102	0	-11	+37	-1	+65	-281
400	0	0	0	0	+65	+47
410	0	0	0	0	+1	-2
302	0	0	0	0	+6	-16
412	0	0	0	0	+6	-4
$V_{jj'}(200)$	0	-3867	+12175	-2	+7182	-12667

$\lambda'\mu'\nu'$ j, j'=	2sσ,2pπ	2pσ,2pσ	2pσ,2pπ	2pπ,2pπ	2p$\bar{\pi}$,2p$\bar{\pi}$
000	0	+3054	0	-724	+724
200	0	+3054	0	-724	+724
100	+2446	+9875	-4220	-2417	+640
300	-460	+319	+1353	-668	+57
101	-398	+319	+178	-668	+57
210	-191	+248	+311	-391	+22
212	+191	+248	-311	-391	+22
102	+42	-271	+37	-60	+22
400	+49	-271	-216	-60	+22
410	-3	+2	+5	-9	0
302	+13	+5	-7	-33	+1
412	+12	+5	-36	-33	+1
$V_{jj'}(200)$	+1702	+16587	-2906	-6179	+2292

TABLE C-5 (contd.)

Potential Integrals: $P_{jj'}(300|\lambda'\mu'\nu')$

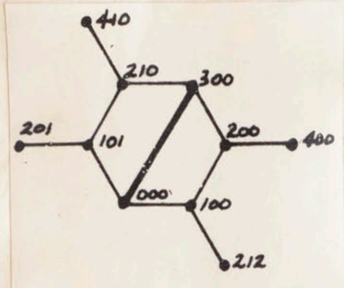

FIG. C-4

$\lambda'\mu'\nu'$ j,j'=	1sσ,1sσ	1sσ,2sσ	1sσ,2pσ	1sσ,2pπ	2sσ,2sσ	2sσ,2pσ
000	0	-1583	+6113	0	+588	-1905
300	0	0	0	0	+588	-603
210	0	0	+1	0	+508	-618
101	0	-8	+29	+2	+508	-1324
100	0	-8	+29	-2	+508	-1324
200	0	0	+1	0	+508	-618
410	0	0	0	0	+9	-5
201	0	0	0	0	+9	-31
212	0	0	0	0	+9	-31
400	0	0	0	0	+9	-5
$V_{jj'}(300)$	0	-1600	+6173	0	+3243	-6465

$\lambda'\mu'\nu'$ j,j'=	2sσ,2pπ	2pσ,2pσ	2pσ,2pπ	2pπ,2pπ	2p$\bar{\pi}$,2p$\bar{\pi}$
000	0	+1607	0	-324	+324
300	0	+1607	0	-324	+324
210	-627	+1473	+1681	-825	+90
101	-564	+1473	+663	-825	+90
100	+564	+1473	-663	-825	+90
200	+627	+1473	-1681	-825	+90
410	-17	+12	+65	-46	+1
201	-19	+12	+10	-46	+1
212	+19	+12	-10	-46	+1
400	+17	+12	-65	-46	+1
$V_{jj'}(300)$	0	+9152	0	-4131	+1014

TABLE C-5 (contd.)

Potential Integrals: $P_{jj'}(400|\lambda'\mu'\nu')$

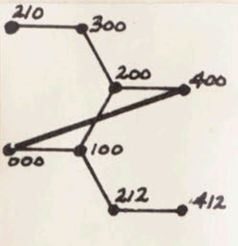

FIG. C-5

$\lambda'\mu'\nu'$	j, j'= 1sσ, 1sσ	1sσ, 2sσ	1sσ, 2pσ	1sσ, 2pπ	2sσ, 2sσ	2sσ, 2pσ
000	0	-179	+1160	0	+72	-382
400	0	0	0	0	+72	-75
200	0	0	0	0	+313	-596
100	0	-1	+7	0	+313	-985
300	0	0	0	0	+27	-59
212	0	0	0	0	+27	-78
210	0	0	0	0	+5	-21
412	0	0	0	0	+5	-7
$V_{jj'}(400)$	0	-180	+1167	0	+835	-2203

$\lambda'\mu'\nu'$	j, j'= 2sσ, 2pπ	2pσ, 2pσ	2pσ, 2pπ	2pπ, 2pπ	$2p\bar{\pi}, 2p\bar{\pi}$	
000	0	+327	0	-48	+48	
400	0	+327	0	-48	+48	
200	-152	+1801	+486	-127	+53	
100	+145	+1801	-272	-127	+53	
300	-47	+157	+136	-97	+6	
212	+49	+157	-105	-97	+6	
210	-14	+25	+18	-32	+1	
412	+10	+25	-45	-32	+1	
$V_{jj'}(400)$	-8	+4619	+217	-606	+217	+217

TABLE C-5 (contd.)

Potential Integrals: $P_{jj'}(500|\lambda'\mu'\nu')$

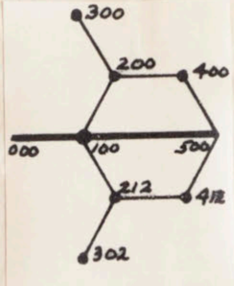

FIG. C-6

$\lambda'\mu'\nu'$ j, j'=	1sσ,1sσ	1sσ,2sσ	1sσ,2pσ	1sσ,2pπ	2sσ,2sσ	2sσ,2pσ
000	(0)	(-53)	(+457)	(0)	(+22)	(-154)
500	(0)	(0)	(0)	(0)	(+22)	(-23)
100	0	0	+3	0	+124	-487
200	0	0	0	0	+42	-118
212	0	0	0	0	+42	-118
400	0	0	0	0	+23	-29
412	0	0	0	0	+23	-29
300	0	0	0	0	+2	-8
302	0	0	0	0	+2	-8
$V_{jj'}(500)$	0	-53	+460	0	+301	-975

$\lambda'\mu'\nu'$ j, j'=	2sσ,2pπ	2pσ,2pσ	2pσ,2pπ	2pπ,2pπ	2p$\bar{\pi}$,2p$\bar{\pi}$
000	(0)	(+133)	(0)	(-17)	(+17)
500	(0)	(+133)	(0)	(-17)	(+17)
100	0	+938	0	-21	+21
200	-51	+315	+144	-75	+9
212	+51	+315	-144	-75	+9
400	-29	+150	+172	-51	+3
412	+29	+150	-172	-51	+3
300	-5	+16	+11	-14	0
302	+5	+16	-11	-14	0
$V_{jj'}(500)$	0	+2164	0	-333	+79

TABLE C-5 (contd.)

Potential Integrals: $P_{jj'}(510|\lambda'\mu'\nu')$

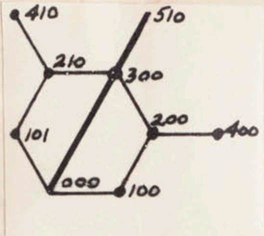

FIG. C-7

$\lambda'\mu'\nu'$ j,j'=	1sσ,1sσ	1sσ,2sσ	1sσ,2pσ	1sσ,2pπ	2sσ,2sσ	2sσ,2pσ
000	(0)	(-53)	(+457)	(0)	(+22)	(-154)
510	(0)	(0)	(0)	(0)	(+22)	(-23)
300	0	0	0	0	+124	-248
200	0	0	0	0	+42	-118
210	0	0	0	0	+42	-118
100	0	0	+2	0	+23	-131
101	0	0	+2	0	+23	-131
400	0	0	0	0	+2	-4
410	0	0	0	0	+2	-4
$V_{jj'}(510)$	0	-53	+461	0	+301	-930

$\lambda'\mu'\nu'$ j,j'=	2sσ,2pπ	2pσ,2pσ	2pσ,2pπ	2pπ,2pπ	2p$\bar{\pi}$,2p$\bar{\pi}$
000	(0)	(+133)	(0)	(-17)	(+17)
510	(0)	(+133)	(0)	(-17)	(+17)
300	0	+938	0	-21	+21
200	+51	+315	-144	-75	+9
210	-51	+315	+144	-75	+9
100	+35	+150	-43	-51	+3
101	-35	+150	+43	-51	+3
400	+4	+16	-20	-14	0
410	-4	+16	+20	-14	0
$V_{jj'}(510)$	0	+2164	0	-333	+79

TABLE C-5 (contd.)

Potential Integrals: $V_{jj'}(600|\lambda'\mu'\nu')$

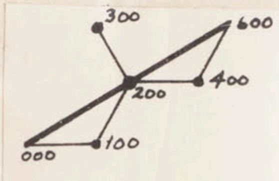

FIG. C-8

$\lambda'\mu'\nu'$ j, j'=	$1s\sigma,1s\sigma$	$1s\sigma,2s\sigma$	$1s\sigma,2p\sigma$	$1s\sigma,2p\pi$	$2s\sigma,2s\sigma$	$2s\sigma,2p\sigma$
000	(0)	(-10)	(+132)	(0)	(+4)	(-46)
600	(0)	(0)	(0)	(0)	(+4)	(-5)
200	0	0	0	0	+31	-101
300	0	0	0	0	+8	-26
400	0	0	0	0	+16	-29
100	0	0	+1	0	+16	-103
$V_{jj'}(600)$	0	-10	+133	0	+80	-309

$\lambda'\mu'\nu'$ j, j'=	$2s\sigma,2p\pi$	$2p\sigma,2p\sigma$	$2p\sigma,2p\pi$	$2p\pi,2p\pi$	$2p\bar{\pi},2p\bar{\pi}$
000	(0)	(+40)	(0)	(-4)	(+4)
600	(0)	(+40)	(0)	(-4)	(+4)
200	0	+318	0	-6	+6
300	-12	+85	+40	-20	+2
400	+12	+176	-79	-15	+2
100	+15	+176	-28	-15	+2
$V_{jj'}(600)$	+16	+835	-67	-64	+21

TABLE C-5 (contd.)

Potential Integrals: $V_{jj'}(700|\lambda'\mu'\nu')$

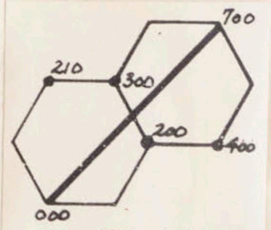

FIG. C-9

$\lambda'\mu'\nu'$ j, j'=	1sσ,1sσ	1sσ,2sσ	1sσ,2pσ	1sσ,2pπ	2sσ,2sσ	2sσ,2pσ
000	(0)	(-6)	(+90)	(0)	(+3)	(-31)
700	(0)	(0)	(0)	(0)	(+3)	(-3)
300	0	0	0	0	+14	-44
200	0	0	0	0	+14	-54
210	0	0	0	0	+2	-14
400	0	0	0	0	+2	-6
$V_{jj'}(700)$	0	-6	+90	0	+38	-152

$\lambda'\mu'\nu'$ j, j'=	2sσ,2pπ	2pσ,2pσ	2pσ,2pπ	2pπ,2pπ	2p$\bar{\pi}$,2p$\bar{\pi}$
000	(0)	(+27)	(0)	(-3)	(+3)
700	(0)	(+27)	(0)	(-3)	(+3)
300	-10	+164	+39	-11	+3
200	+11	+164	-33	-11	+3
210	-5	+31	+13	-10	+1
400	+4	+31	-24	-10	+1
$V_{jj'}(700)$	-1	+445	-5	-48	+13

TABLE C-5 (contd.)

Pontential Integrals: $V_{jj'}(800|\lambda'\mu'\nu')$

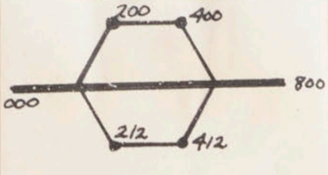

FIG. C-10

$\lambda'\mu'\nu'$ j,j′=	$1s\sigma,1s\sigma$	$1s\sigma,2s\sigma$	$1s\sigma,2p\sigma$	$1s\sigma,2p\pi$	$2s\sigma,2s\sigma$	$2s\sigma,2p\sigma$
000	(0)	(-2)	(+31)	(0)	(+1)	(-11)
800	(0)	(0)	(0)	(0)	(+1)	(-1)
400	0	0	0	0	+2	-5
200	0	0	0	0	+2	-12
212	0	0	0	0	+2	-12
412	0	0	0	0	+2	-5
$V_{jj'}(800)$	0	-2	+31	0	+9	-46

$\lambda'\mu'\nu'$ j,j′=	$2s\sigma,2p\pi$	$2p\sigma,2p\sigma$	$2p\sigma,2p\pi$	$2p\pi,2p\pi$	$2p\bar{\pi},2p\bar{\pi}$
000	(0)	(+10)	(0)	(-1)	(+1)
800	(0)	(+10)	(0)	(-1)	(+1)
400	-2	+32	+15	-5	0
200	-3	+32	+9	-5	0
212	+3	+32	-9	-5	0
412	+2	+32	-15	-5	0
$V_{jj'}(800)$	0	+146	0	-21	+4

TABLE C-5 (contd.)

Potential Integrals: $V_{dd}^{jj'}(900|\lambda'\mu'\nu')$

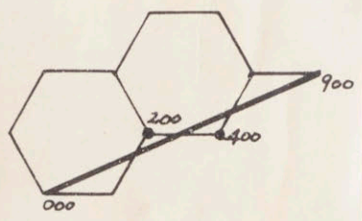

FIG. C-11

$\lambda'\mu'\nu'$ j, j'=	$1s\sigma,1s\sigma$	$1s\sigma,2s\sigma$	$1s\sigma,2p\sigma$	$1s\sigma,2p\pi$	$2s\sigma,2s\sigma$	$2s\sigma,2p\sigma$
000	(0)	(0)	(+12)	(0)	(0)	(-4)
900	(0)	(0)	(0)	(0)	(0)	(0)
200	0	0	0	0	+2	-10
400	0	0	0	0	+2	-5
$V_{dd}^{jj'}(900)$	0	0	+12	0	+3	-19

$\lambda'\mu'\nu'$ j, j'=	$2s\sigma,2p\pi$	$2p\sigma,2p\sigma$	$2p\sigma,2p\pi$	$2p\pi,2p\pi$	$2p\bar{\pi},2p\bar{\pi}$
000	(0)	(+4)	(0)	(0)	(0)
900	(0)	(+4)	(0)	(0)	(0)
200	-1	+32	+2	-1	0
400	0	+32	-3	-1	0
$V_{dd}^{jj'}(900)$	0	+71	-1	-2	+1

TABLE C-6

Hamiltonian integrals computed from the kinetic energy integrals of table C-2 and the potential integrals of table C-5. These integrals which were used (along with the overlap integrals of table C-2) for the solution of figures 7-1 and 7-2, depend only on $\lambda\mu$ and are listed in a square matrix of vectors where each vector represents the integrals for the values $\lambda\mu$ = 00, 10, 20, 30, 40, 50, 51, 60, 70, 80, 90. Non-significant zeros are omitted for legibility. Energy units are two Rydbergs.

Hamiltonian Integrals: $H_{jj'}(\lambda\mu\nu)$

$j \backslash j'$	$1s\sigma'$	$2s\sigma'$	$2p\sigma'$	$2p\pi'$	$2p\bar{\pi}'$
$1s\sigma$	-7.85579	+.33201	+.00000	+.00000	+.00000
	-. 94	+.40135	-.75465	0	0
	0	+. 4065	-.12420	+. 2	0
	0	+. 1694	-. 6329	0	0
	0	+. 193	-. 1208	0	0
	0	+. 57	-. 478	0	0
	0	+. 57	-. 479	0	0
	0	+. 11	-. 139	0	0
	0	+. 7	-. 94	0	0
	0	+. 2	-. 32	0	0
	0	0	-. 12	0	0
$2s\sigma$	+.33201	-.24006	+.00000	+.00000	+.00000
	+.40135	-.21981	+.18204	0	0
	+. 4065	-. 8383	+.12138	-. 1702	0
	+. 1694	-. 4249	+. 6858	0	0
	+. 193	-. 1172	+. 2657	+. 8	0
	+. 57	-. 455	+. 1251	0	0
	+. 57	-. 455	+. 1207	0	0
	+. 11	-. 129	+. 431	-. 16	0
	+. 7	-. 73	+. 244	+. 1	0
	+. 2	-. 21	+. 86	0	0
	0	-. 8	+. 38	0	0

TABLE C-6 (cont.)

Hamiltonian Integrals (cont.): $H_{jj'}(\lambda\mu\nu)$

$j \backslash j'$	$1s\sigma$	$2s\sigma$	$2p\sigma$	$2p\pi$	$2p\bar{\pi}$
$2p\sigma$	+.00000	+.00000	+.09046	+.00000	+.00000
	-.75465	+.18204	-. 1718	0	0
	-.12420	+.12138	-.12470	+. 2906	0
	-. 6329	+. 6858	-. 7551	0	0
	-. 1208	+. 2657	-. 4789	-. 218	0
	-. 479	+. 1207	-. 2407	0	0
	-. 478	+. 1251	-. 2407	0	0
	-. 139	+. 431	-. 1002	+. 67	0
	-. 94	+. 244	-. 584	+. 5	0
	-. 32	+. 86	-. 223	0	0
	-. 12	+. 38	-. 112	+. 1	0
$2p\pi$	+.00000	+.00000	+.00000	+.09046	+.00000
	0	0	0	+.12197	0
	-. 2	+. 1702	-. 2906	+. 5768	0
	0	0	0	+. 4139	0
	0	-. 8	+. 218	+. 713	0
	0	0	0	+. 401	0
	0	0	0	+. 401	0
	0	+. 16	-. 67	+. 94	0
	0	-. 1	-. 5	+. 71	0
	0	0	0	+. 31	0
	0	0	-. 1	+. 7	0
$2p\bar{\bar{\pi}}$	+.00000	+.00000	+.00000	+.00000	+.17747
	0	0	0	0	-. 5317
	0	0	0	0	-. 1880
	0	0	0	0	-. 1022
	0	0	0	0	-. 323
	0	0	0	0	-. 146
	0	0	0	0	-. 146
	0	0	0	0	-. 51
	0	0	0	0	-. 36
	0	0	0	0	-. 14
	0	0	0	0	-. 6

A CALCULATION OF THE ENERGY BANDS OF THE GRAPHITE CRYSTAL BY MEANS OF THE TIGHT-BINDING METHOD

by

FERNANDO JOSÉ CORBATÓ

B. S. California Institute of Technology

(1950)

Volume 2 of 2 Volumes

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at the

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

September 1956

Signature redacted

Signature of Author. . . . .
Department of Physics, August 20, 1956

Signature redacted

Certified by . . . .
Thesis Supervisor

Signature redacted

Accepted by . . . .
Chairman, Departmental Committee
on Graduate Students

Appendix D

Numerical Results

The following 100 microfilm prints give the numerical results of the most accurate solutions indicated in part by fig. 7-1. The first set of 25 prints gives the $\mathcal{H}_{ij}(\vec{k})$ and $\mathcal{S}_{ij}(\vec{k})$ matrices of the π states. The second set of 25 prints gives the corresponding matrices of the σ state solutions. The third and fourth sets of 25 prints give the $E_\ell(\vec{k})$ and $C_{i\ell}(\vec{k})$ solutions of the π and σ states, respectively. The matrix element $\mathcal{M}_{ij}$ is taken to be the element of the <u>ith</u> row and the <u>jth</u> column. The basis states for the matrices are:

	Basis state	Bloch wave subscript
π states:	1	2pz, + 1
	2	2pz, - 1
σ states	1	2s, + 1
	2	2s, - 1
	3	2px, + 1
	4	2px, - 1
	5	2py, + 1
	6	2py, - 1
	7	1s, + 1
	8	1s, - 1

The wave vector points for which solutions are given are indicated by fig. D-1.

The numbered wave vector points of fig. D-1 are associated with identifying code numbers indicating different computer runs; the unprimed and primed point numbers refer to solutions with code numbers 1099 and 1299, respectively.

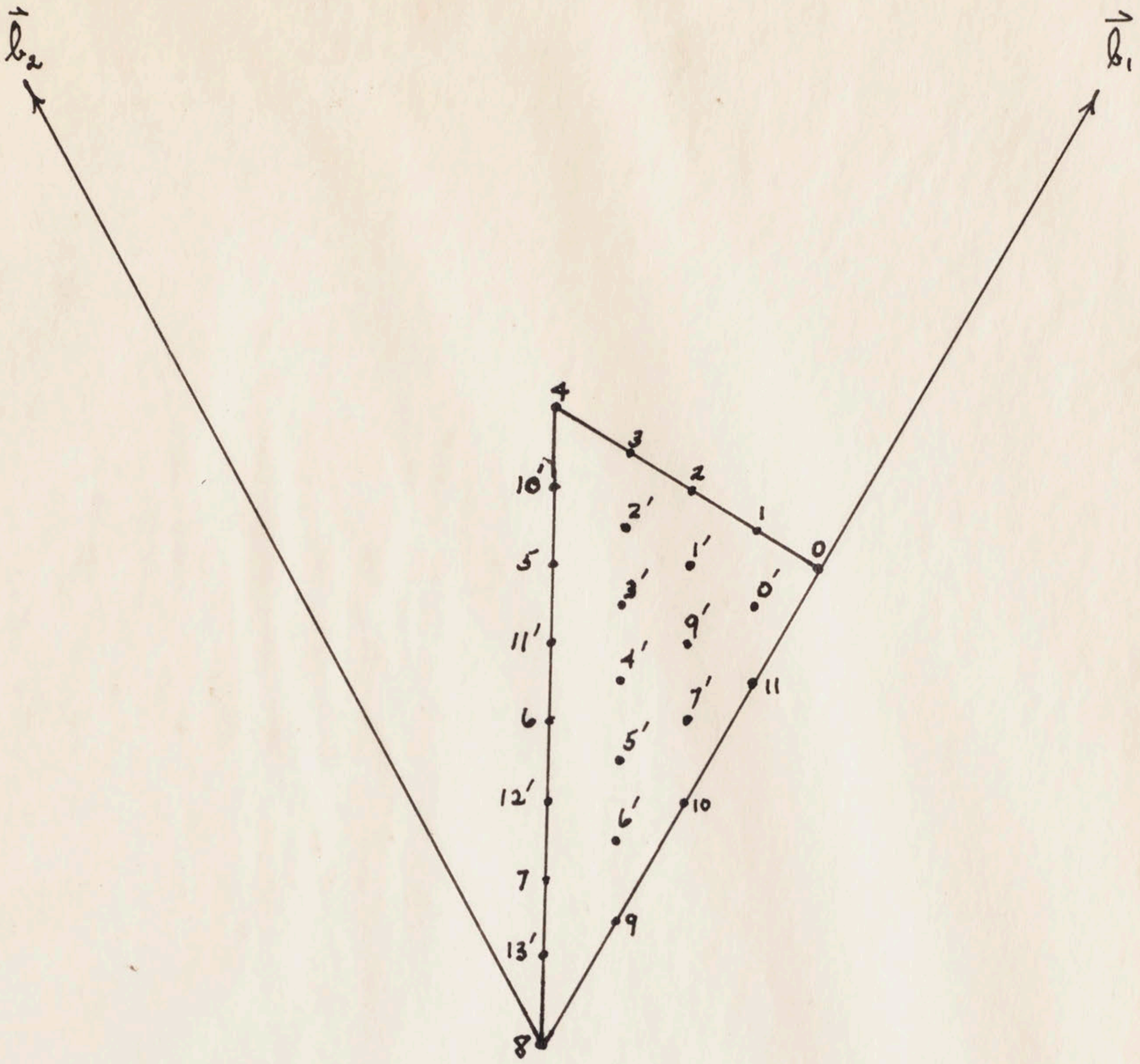


Fig D-1
Wave Vector Points of the Numerical Results

Every matrix and solution has an identifying heading block of three rows which always has a code number (first row, first column), a point number (second row, first column) and a blank space (first row, fourth column). (In the prints, +.10990000/+04 means +.1099 x 10^4.) The various heading blocks are illustrated where k_1 and k_2 are the wave vector components as defined in eq. 2-5c.

Hamiltonian matrix heading:

Code no.	-30		
Point no.	9	9	
	96	$96k_1$	$96k_2$

Overlap matrix heading:

Code no.		-30	
Point no.	9	9	
	96	$96k_1$	$96k_2$

Solution heading:

Code no.	-30	-30	
Point no.	9	9	
	96	$96k_1$	$96k_2$

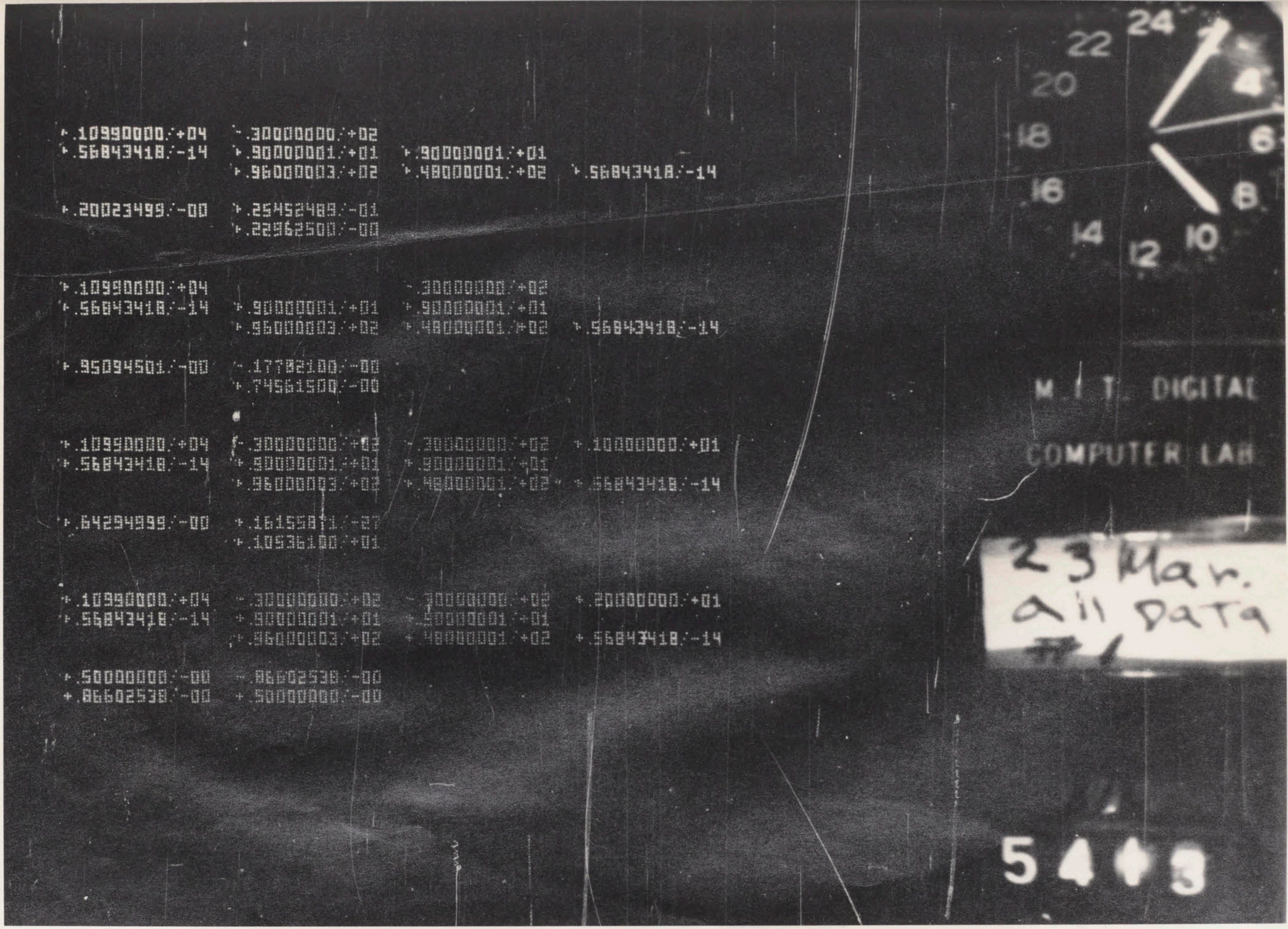
All other forms of heading blocks (present only in π state prints) are for internal check results.

The $\mathcal{H}$ and $\mathcal{S}$ matrices, which are given in a symmetric matrix display form, are found at the top of the appropriate print in all cases. The solutions are given as consecutive vectors left-to-right, row-after-row with the sequence of: the eigenvalues as a vector, a blank vector, the first eigenvector, the second eigenvector, etc. The σ state solutions start from the top of the appropriate print and the

π state solutions are found at the bottom.

To avoid ambiguity, the following chart of frame numbers is given:

	π states		σ states	
Point number	$\mathcal{H},\mathcal{S}$	E, C	$\mathcal{H},\mathcal{S}$	E, C
0	5413	5414	5443	5448
1	5415	5416	5449	5454
2	5417	5418	5455	5460
3	5419	5420	5461	5466
4	5421	5422	5467	5472
5	5423	5424	5473	5478
6	5425	5426	5479	5484
7	5427	5428	5485	5490
8	5429	5430	5491	5496
9	5431	5432	5497	5502
10	5433	5434	5503	5508
11	5435	5436	5509	5514
0'	9473	9474	9507	9512
1'	9475	9476	9513	9518
2'	9477	9478	9519	9524
3'	9479	9480	9525	9530
4'	9481	9730	9531	9536
5'	9483	9484	9537	9542
6'	9485	9486	9543	9548
7'	9487	9488	9549	9554
9'	9491	9492	9561	9566
10'	9493	9494	9567	9572
11'	9495	9496	9573	9578
12'	9497	9498	9579	9584
13'	9499	9500	9585	9590



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                 +.22962500/-00

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23 Mar.
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+.10990000./+04                      .30000000./+02
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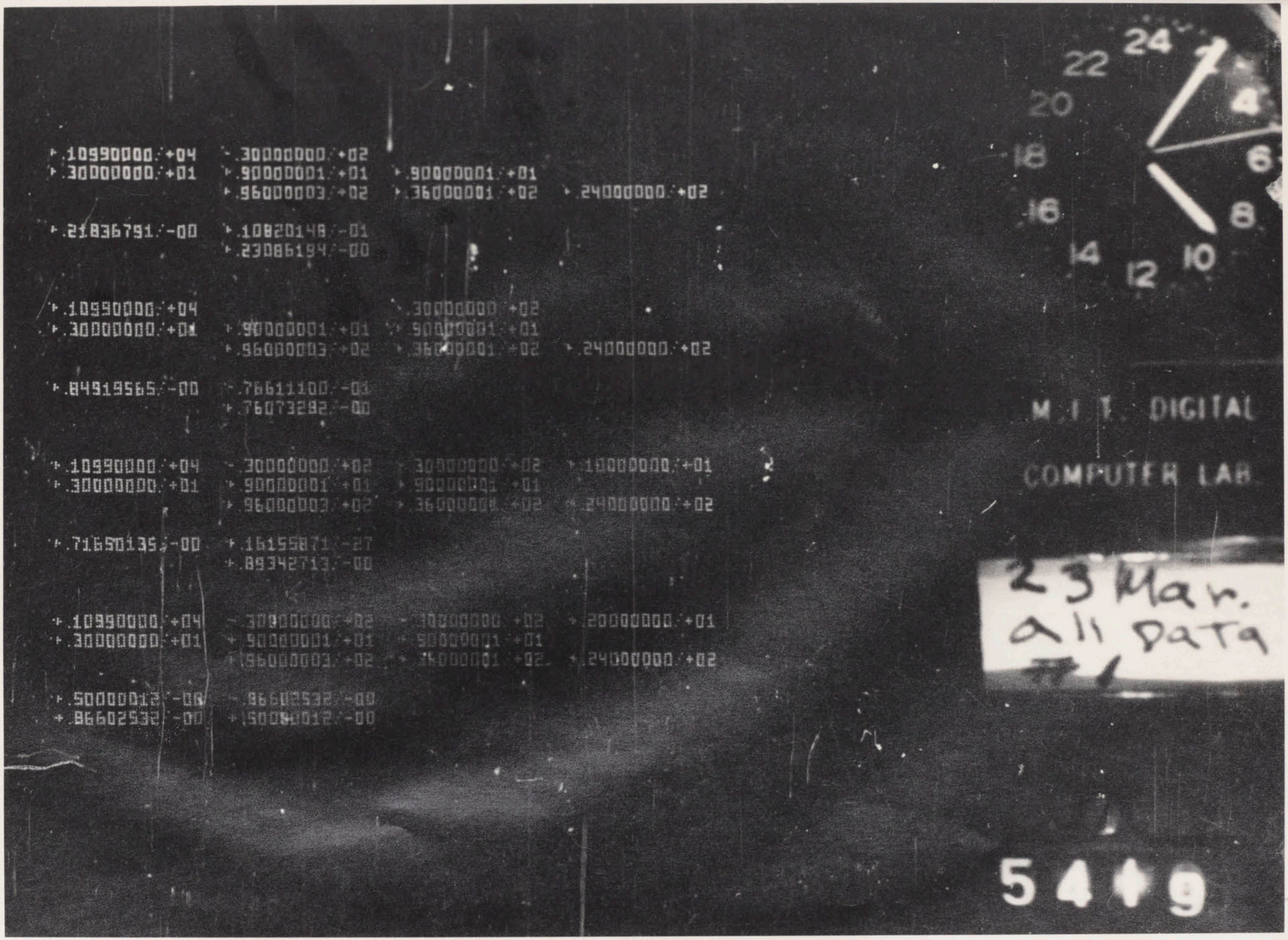

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                  +.96000003./+02   +.36000001./+02   +.24000000./+02

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23 Mar.
all Data
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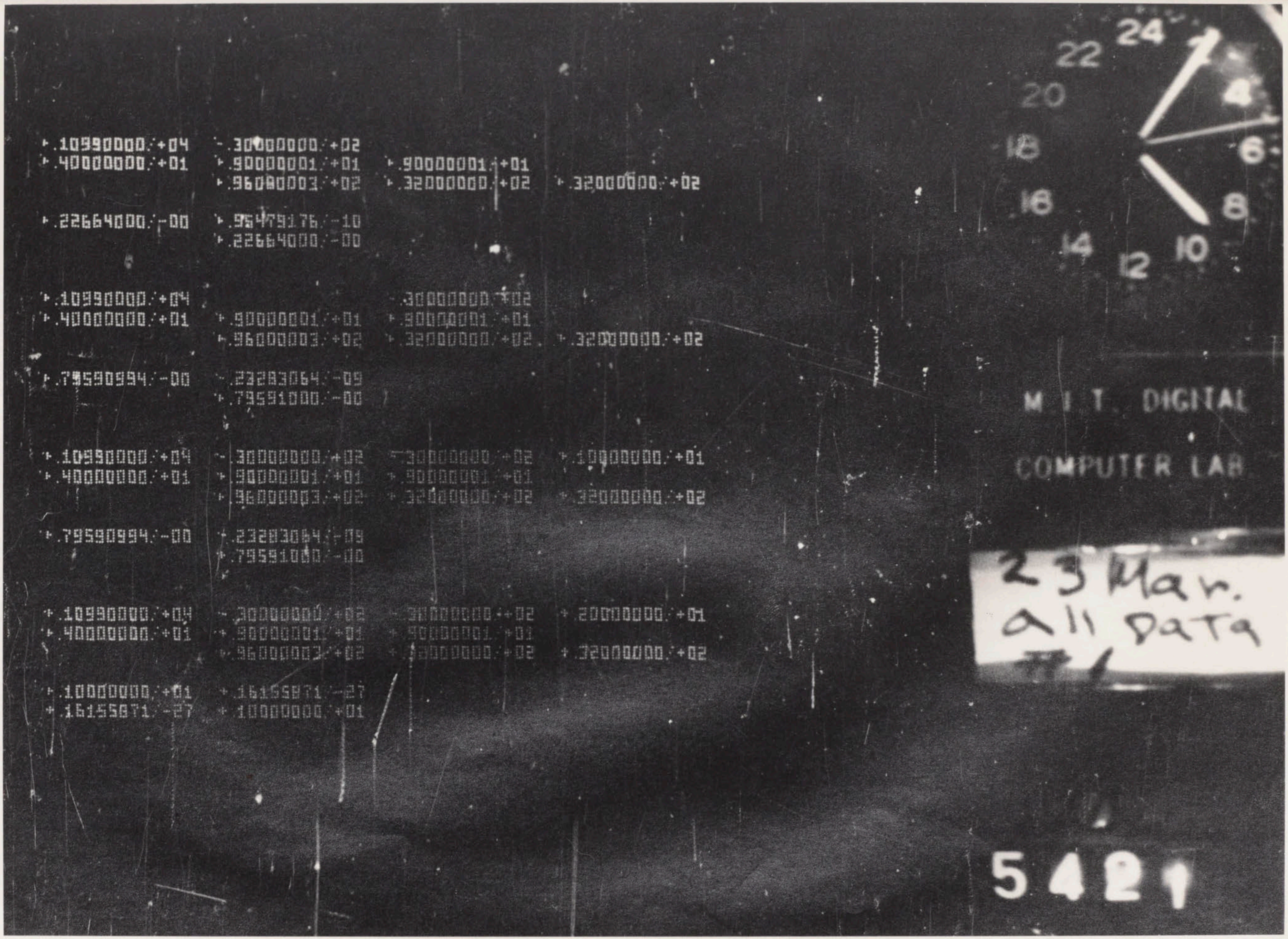

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                  +.22664000./-00


+.10990000./+04                     -.30000000./+02
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                  +.79591000./-00


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+.40000000./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.32000000./+02   +.32000000./+02

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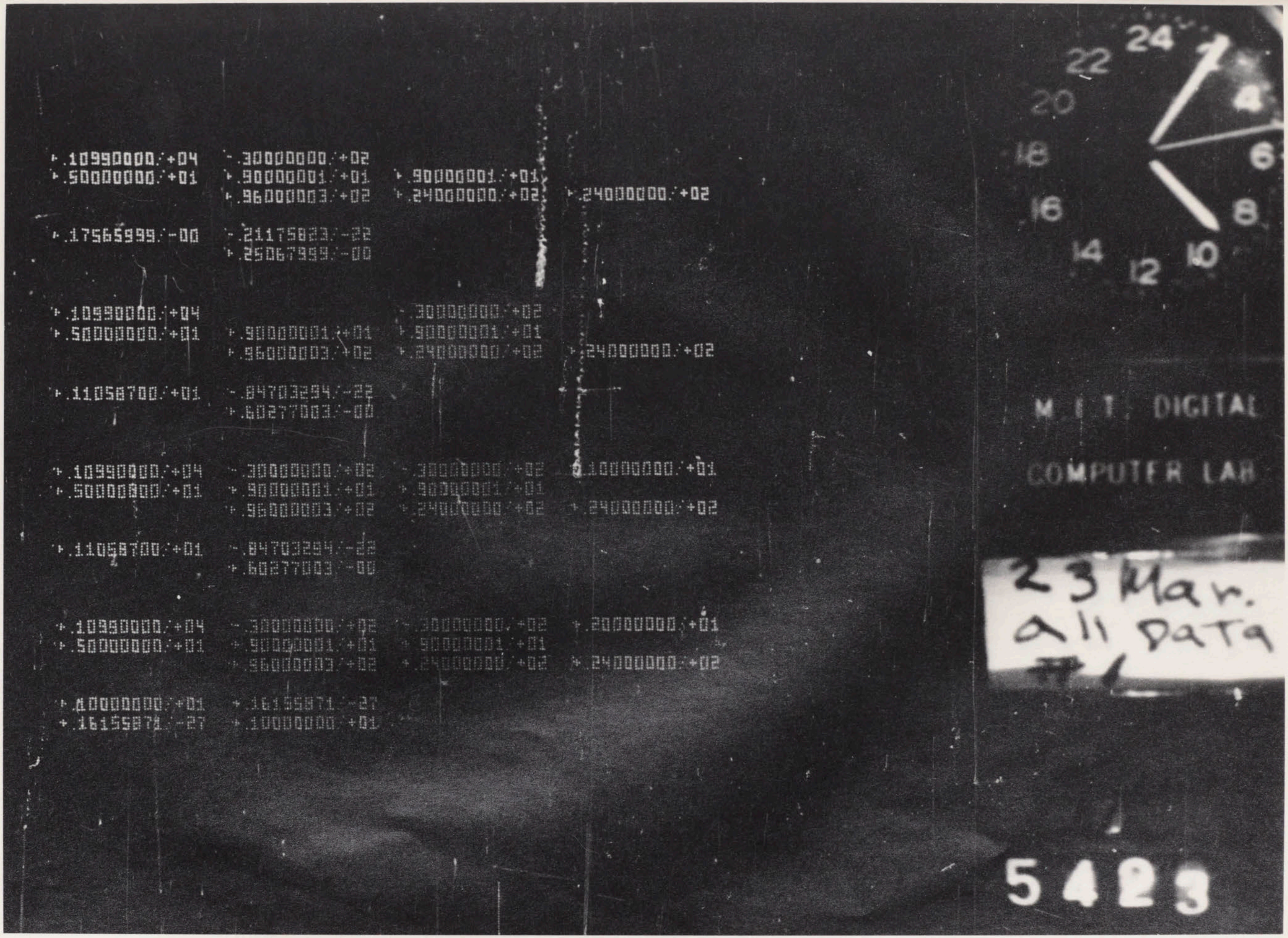

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                  +.25067999./-00


+.10990000./+04                     -.30000000./+02
+.50000000./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.24000000./+02   +.24000000./+02

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+.10990000./+04   -.30000000./+02   -.30000000./+02   +.10000000./+01
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+.10000000./+01   +.16155871./-27
+.16155871./-27   +.10000000./+01
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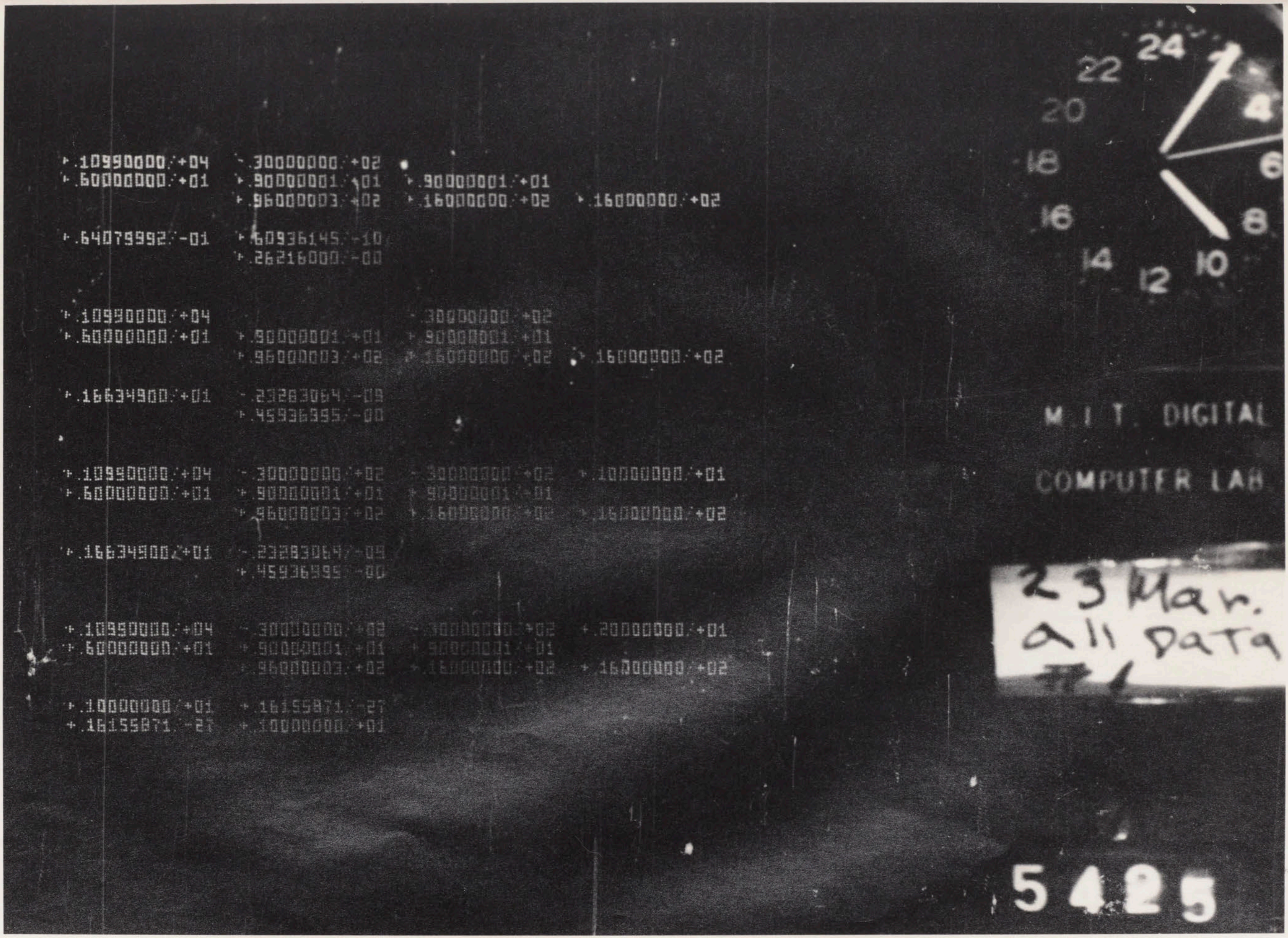
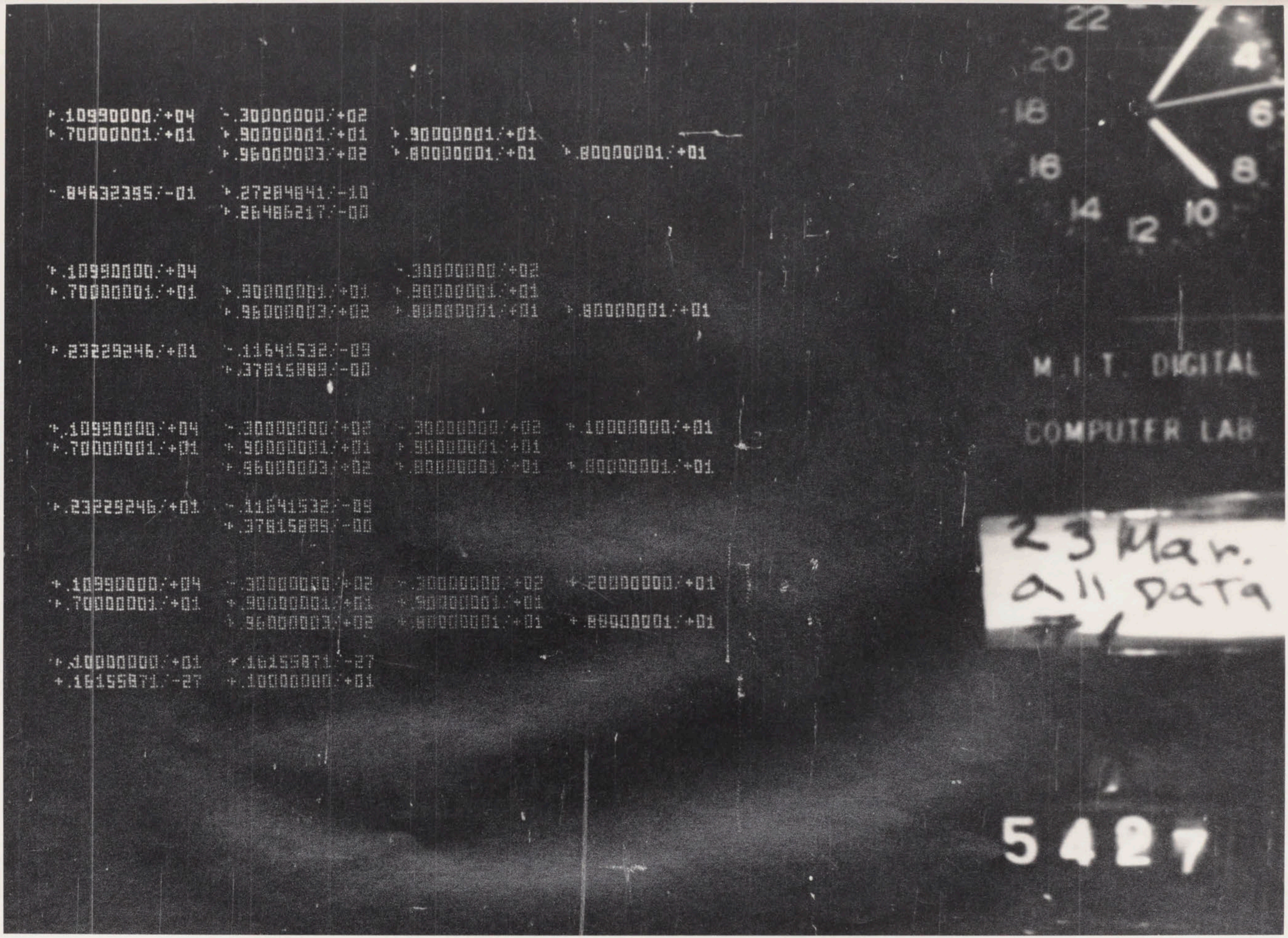
#1

5423



```
+.10990000/+04  -.30000000/+02
+.60000000/+01  +.90000001/+01  +.90000001/+01
                +.96000003/+02  +.16000000/+02  +.16000000/+02

+.64079992/-01  +.60936145/-10
                +.26216000/-00


+.10990000/+04                  -.30000000/+02
+.60000000/+01  +.90000001/+01  +.90000001/+01
                +.96000003/+02  +.16000000/+02  +.16000000/+02

+.16634900/+01  -.23283064/-09
                +.45936395/-00


+.10990000/+04  -.30000000/+02  -.30000000/+02  +.10000000/+01
+.60000000/+01  +.90000001/+01  +.90000001/+01
                +.96000003/+02  +.16000000/+02  +.16000000/+02

+.16634900/+01  -.23283069/-09
                +.45936995/-00


+.10990000/+04  -.30000000/+02  -.30000000/+02  +.20000000/+01
+.60000000/+01  +.90000001/+01  +.90000001/+01
                +.96000003/+02  +.16000000/+02  +.16000000/+02

+.10000000/+01  +.16155871/-27
+.16155871/-27  +.10000000/+01
```



```
+.10990000/+04   -.30000000/+02
+.70000001/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.80000001/+01   +.80000001/+01

-.84632395/-01   +.27284841/-10
                 +.26486217/-00


+.10990000/+04                    -.30000000/+02
+.70000001/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.80000001/+01   +.80000001/+01

+.23229246/+01   -.11641532/-09
                 +.37815889/-00


+.10990000/+04   -.30000000/+02   -.30000000/+02   +.10000000/+01
+.70000001/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.80000001/+01   +.80000001/+01

+.23229246/+01   -.11641532/-09
                 +.37815885/-00


+.10990000/+04   -.30000000/+02   -.30000000/+02   +.20000000/+01
+.70000001/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.80000001/+01   +.80000001/+01

+.10000000/+01   +.16155871/-27
+.16155871/-27   +.10000000/+01
```

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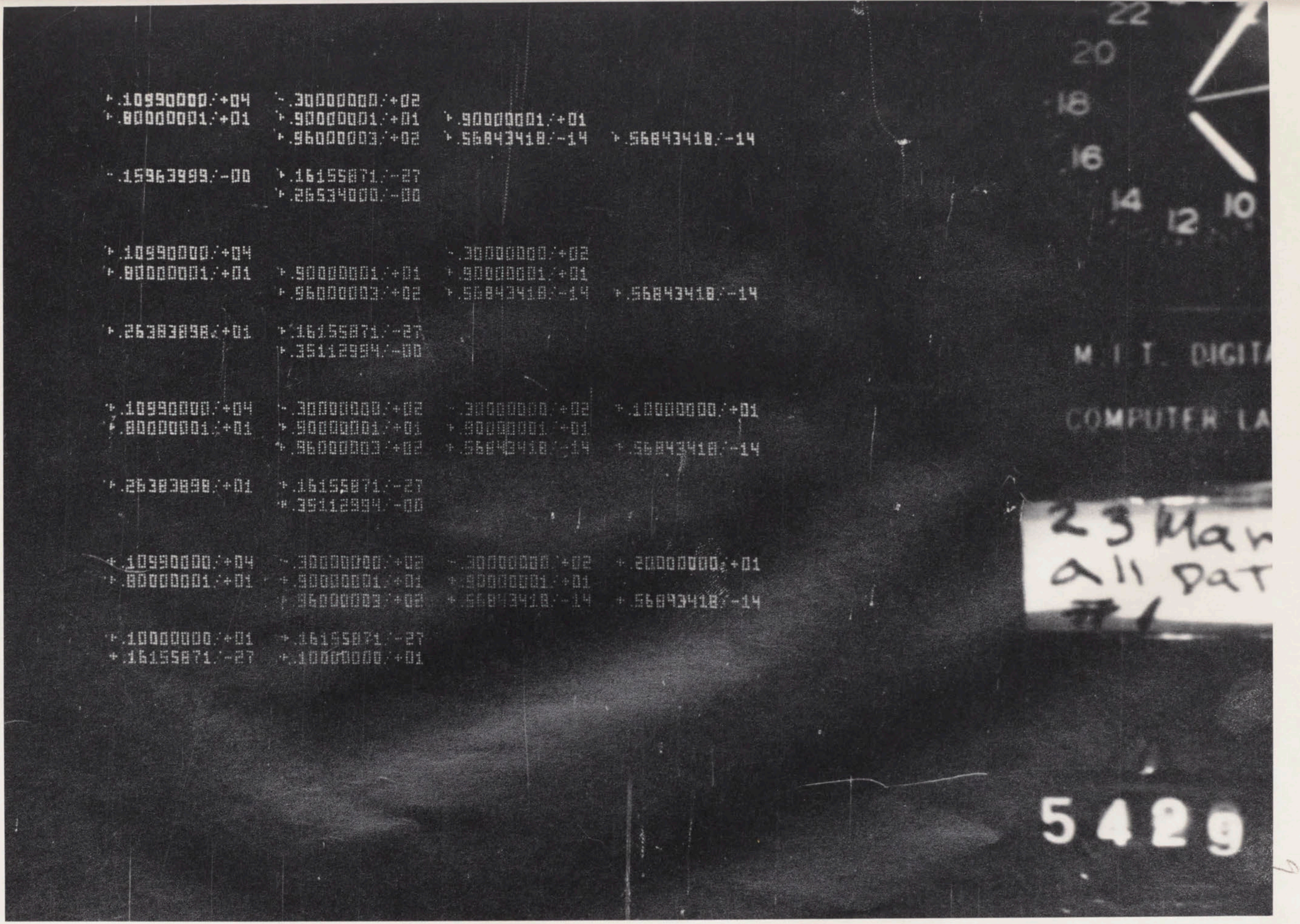
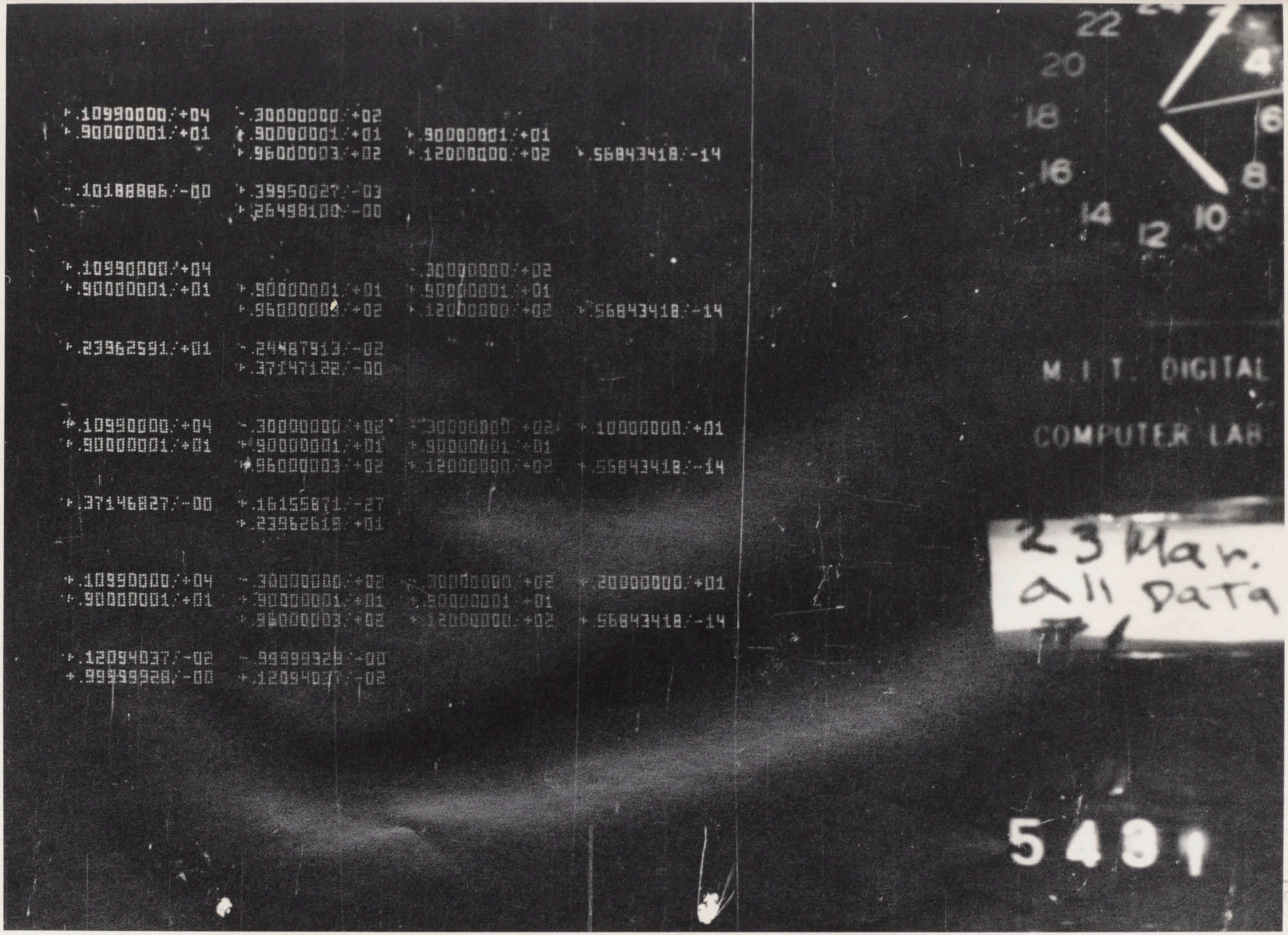
23 Mar.
all Data
#1

5427



```
+.10990000/+04   -.30000000/+02
+.80000001/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.56843418/-14   +.56843418/-14

-.15963999/-00   +.16155871/-27
                 +.26534000/-00


+.10990000/+04                    -.30000000/+02
+.80000001/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.56843418/-14   +.56843418/-14

+.26383898/+01   +.16155871/-27
                 +.35112994/-00


+.10990000/+04   -.30000000/+02   -.30000000/+02   +.10000000/+01
+.80000001/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.56843418/-14   +.56843418/-14

+.26383898/+01   +.16155871/-27
                 +.35112994/-00


+.10990000/+04   -.30000000/+02   -.30000000/+02   +.20000000/+01
+.80000001/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.56843418/-14   +.56843418/-14

+.10000000/+01   +.16155871/-27
+.16155871/-27   +.10000000/+01
```



```
+.10990000/+04   -.30000000/+02
+.90000001/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.12000000/+02   +.56843418/-14

-.10188886/-00   +.39950027/-03
                 +.26498100/-00


+.10990000/+04                    -.30000000/+02
+.90000001/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.12000000/+02   +.56843418/-14

+.23962591/+01   -.24487913/-02
                 +.37147122/-00


+.10990000/+04   -.30000000/+02   -.30000000/+02   +.10000000/+01
+.90000001/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.12000000/+02   +.56843418/-14

+.37146827/-00   +.16155871/-27
                 +.23962619/+01


+.10990000/+04   -.30000000/+02   -.30000000/+02   +.20000000/+01
+.90000001/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.12000000/+02   +.56843418/-14

+.12094037/-02   -.99999920/-00
+.99999928/-00   +.12094037/-02
```

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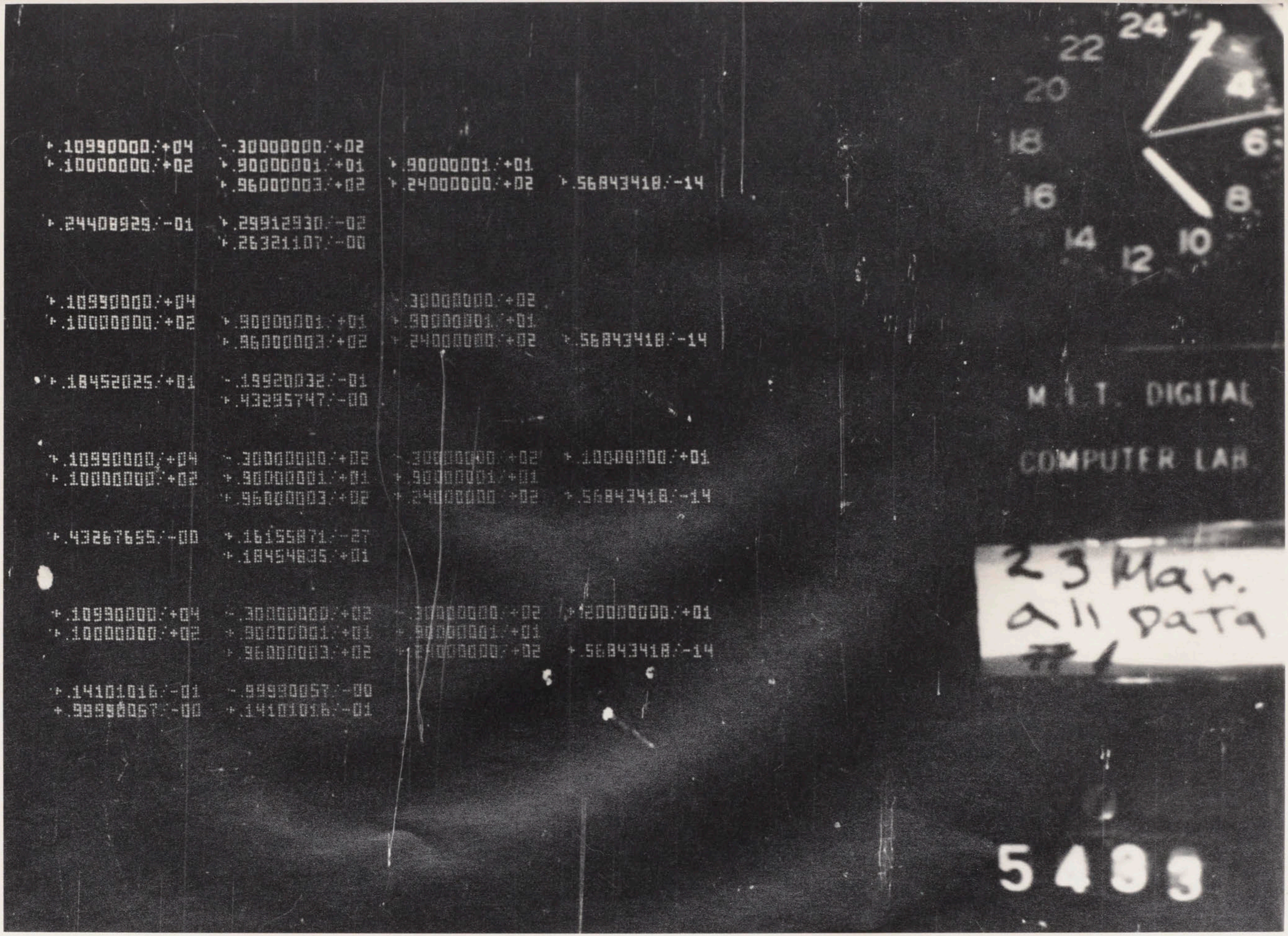
all Data
#1

5481



```
+.10990000/+04   -.30000000/+02
+.10000000/+02   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.24000000/+02   +.56843418/-14

+.24408929/-01   +.29912930/-02
                 +.26321107/-00


+.10990000/+04                    -.30000000/+02
+.10000000/+02   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.24000000/+02   +.56843418/-14

+.18452025/+01   -.19920032/-01
                 +.43295747/-00


+.10990000/+04   -.30000000/+02   -.30000000/+02   +.10000000/+01
+.10000000/+02   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.24000000/+02   +.56843418/-14

+.43267655/-00   +.16155871/-27
                 +.18454835/+01


+.10990000/+04   -.30000000/+02   -.30000000/+02   +.20000000/+01
+.10000000/+02   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.24000000/+02   +.56843418/-14

+.14101016/-01   -.99990057/-00
+.99990067/-00   +.14101016/-01
```

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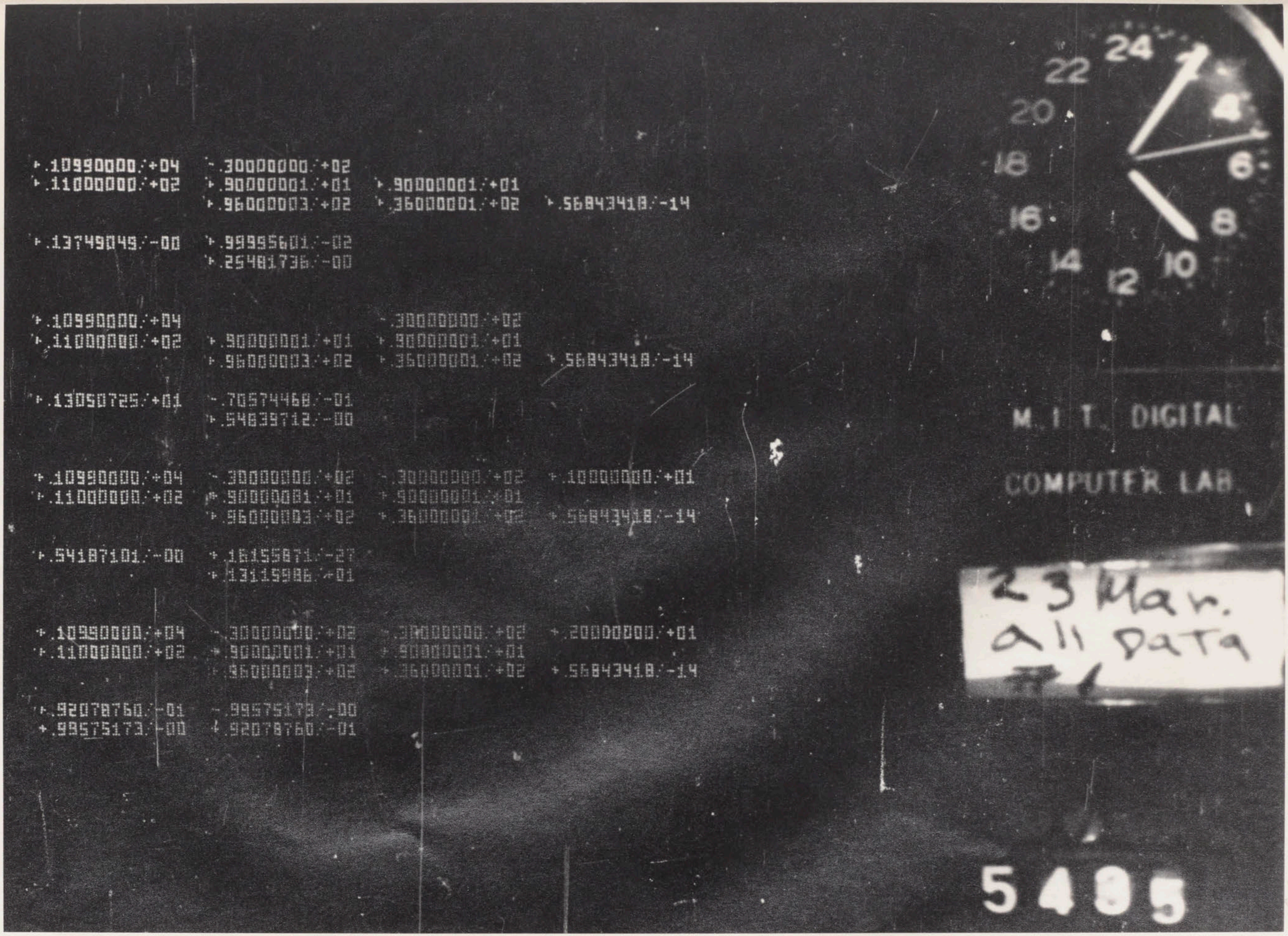
23 Mar.
all data

5483



```
+.10990000./+04  -.30000000./+02
+.11000000./+02  +.90000001./+01  +.90000001./+01
                 +.96000003./+02  +.36000001./+02  +.56843418./-14

+.13749049./-00  +.99955601./-02
                 +.25481736./-00


+.10990000./+04                   -.30000000./+02
+.11000000./+02  +.90000001./+01  +.90000001./+01
                 +.96000003./+02  +.36000001./+02  +.56843418./-14

+.13050725./+01  -.70574468./-01
                 +.54839712./-00


+.10990000./+04  -.30000000./+02  -.30000000./+02  +.10000000./+01
+.11000000./+02  +.90000001./+01  +.90000001./+01
                 +.96000003./+02  +.36000001./+02  +.56843418./-14

+.54187101./-00  +.16155871./-27
                 +.13115986./-01


+.10990000./+04  -.30000000./+02  -.30000000./+02  +.20000000./+01
+.11000000./+02  +.90000001./+01  +.90000001./+01
                 +.96000003./+02  +.36000001./+02  +.56843418./-14

+.92078760./-01  -.99575173./-00
+.99575173./-00  +.92078760./-01
```

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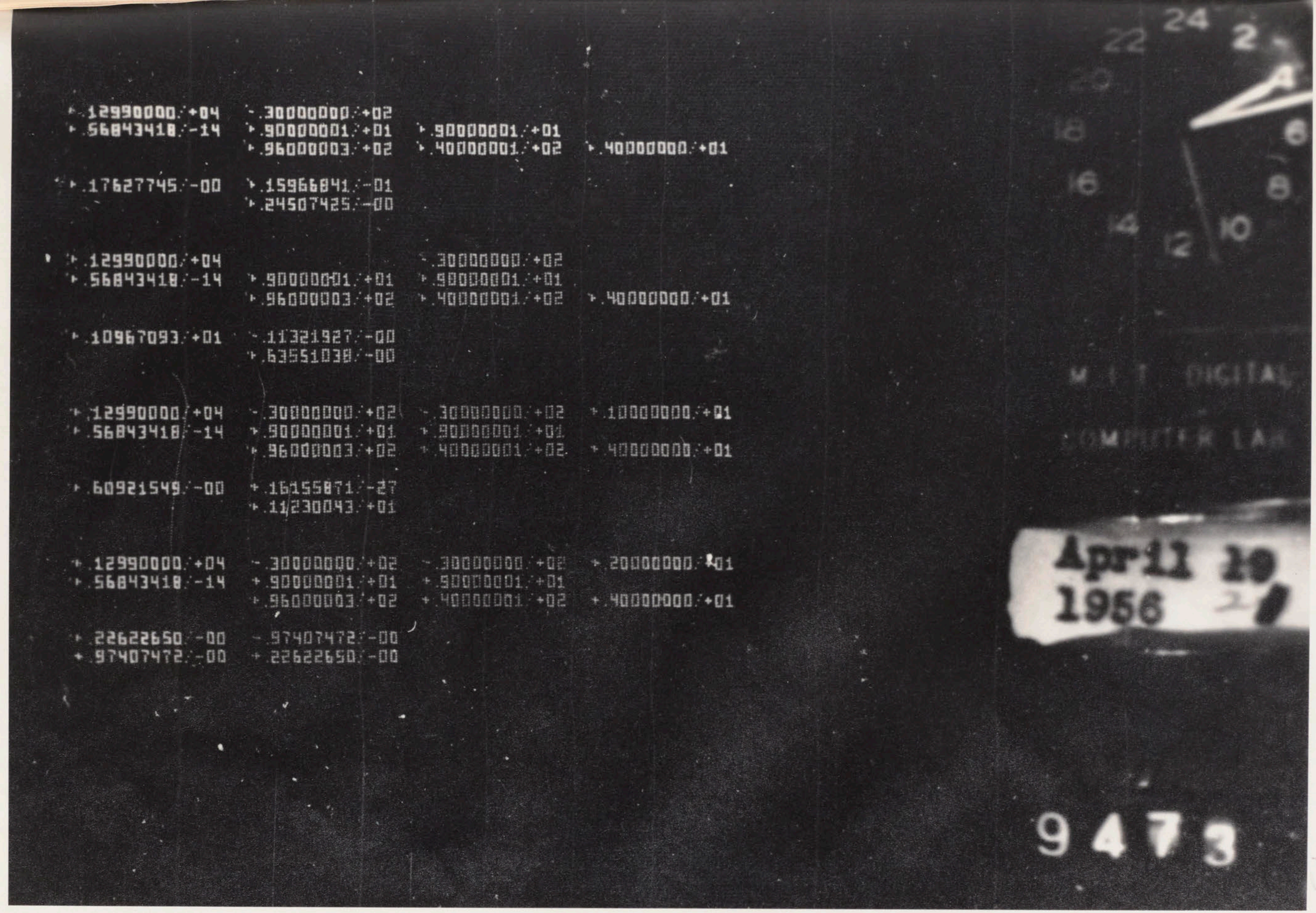
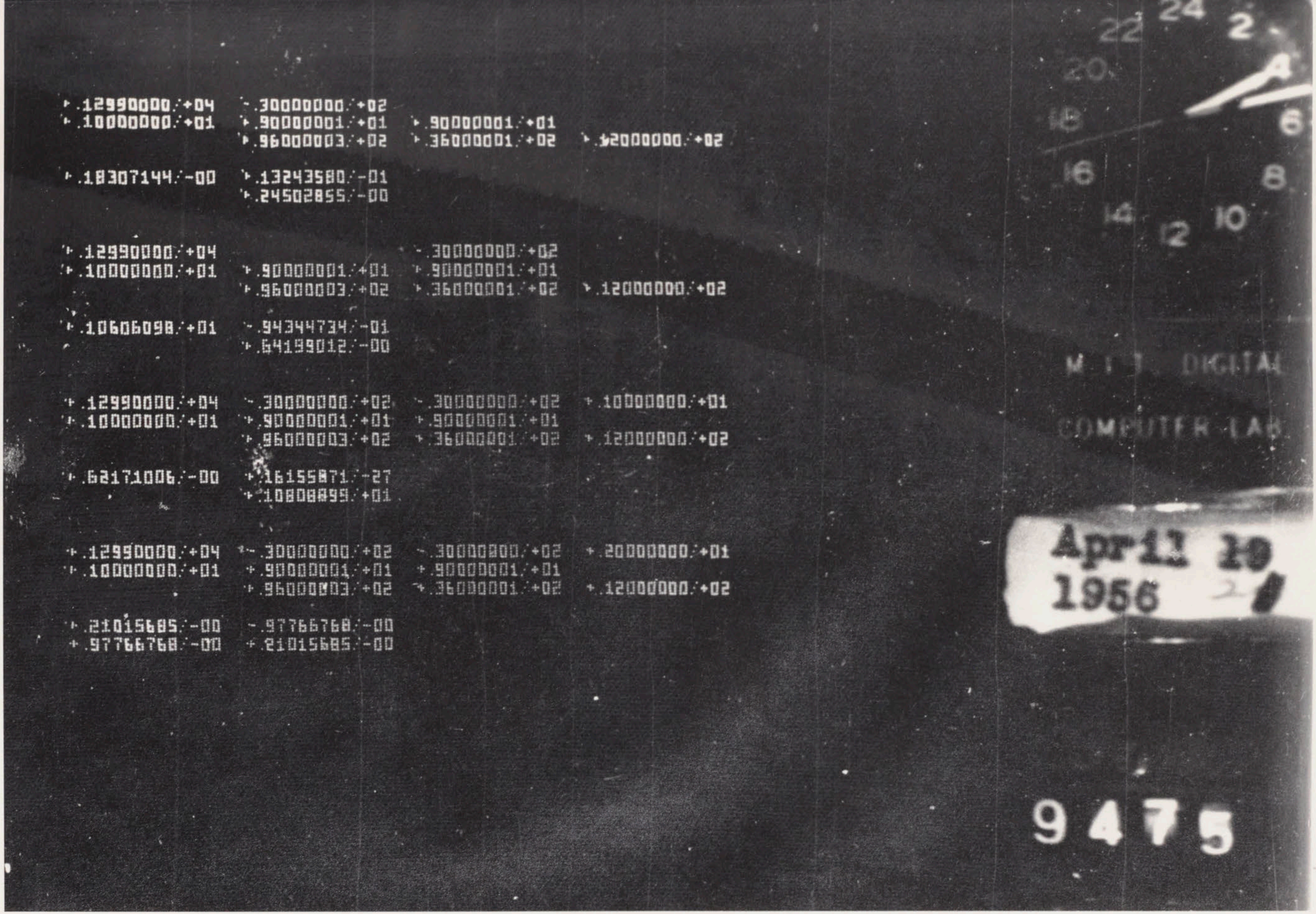
23 Mar.
all Data
#1

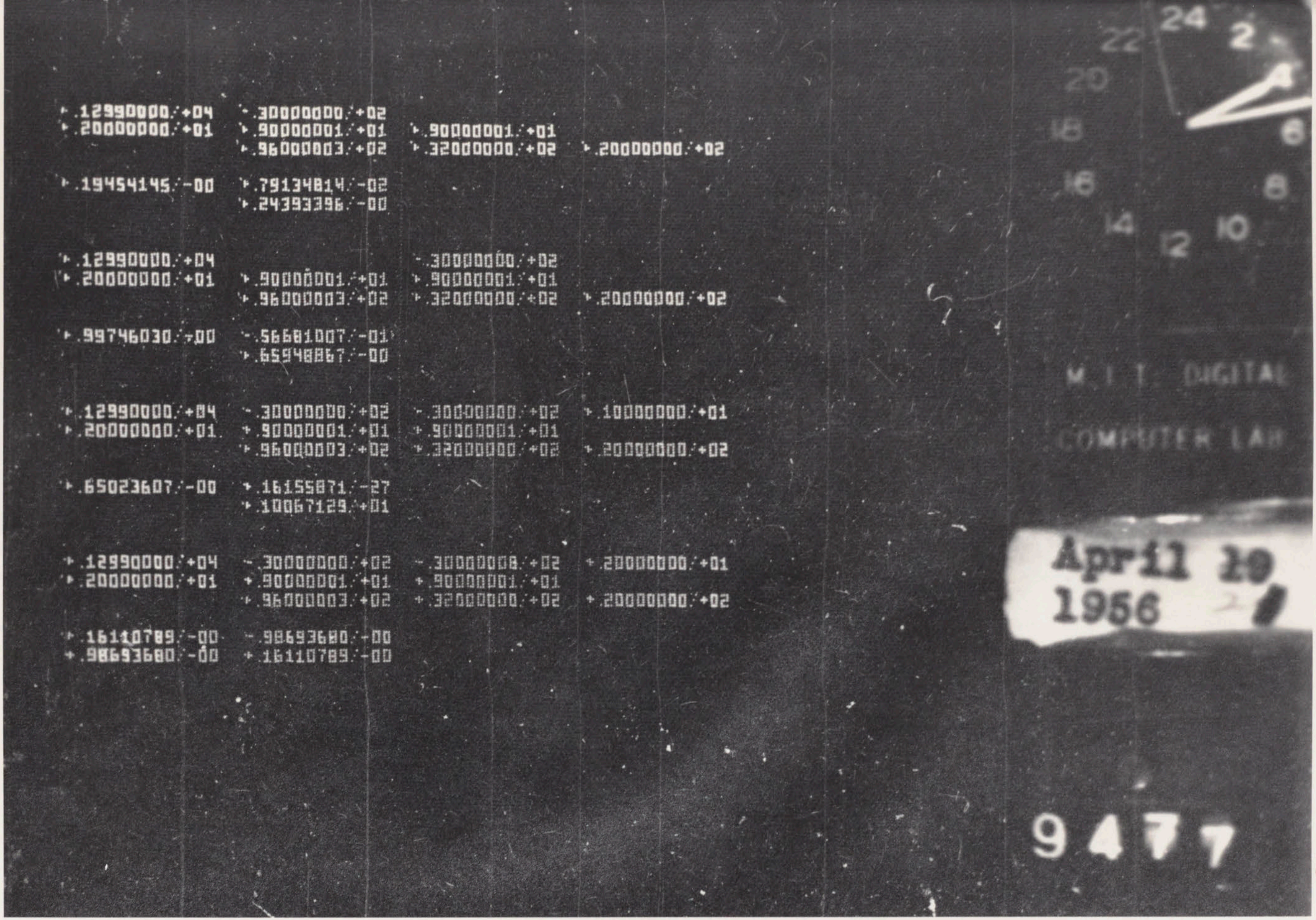
5485



```
+.12990000/+04   -.30000000/+02
+.56843418/-14   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.40000001/+02   +.40000000/+01

+.17627745/-00   +.15966841/-01
                 +.24507425/-00

+.12990000/+04                    -.30000000/+02
+.56843418/-14   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.40000001/+02   +.40000000/+01

+.10967093/+01   -.11321927/-00
                 +.63551038/-00

+.12990000/+04   -.30000000/+02   -.30000000/+02   +.10000000/+01
+.56843418/-14   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.40000001/+02   +.40000000/+01

+.60921549/-00   +.16155871/-27
                 +.11230043/+01

+.12990000/+04   -.30000000/+02   -.30000000/+02   +.20000000/+01
+.56843418/-14   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.40000001/+02   +.40000000/+01

+.22622650/-00   -.97407472/-00
+.97407472/-00   +.22622650/-00
```

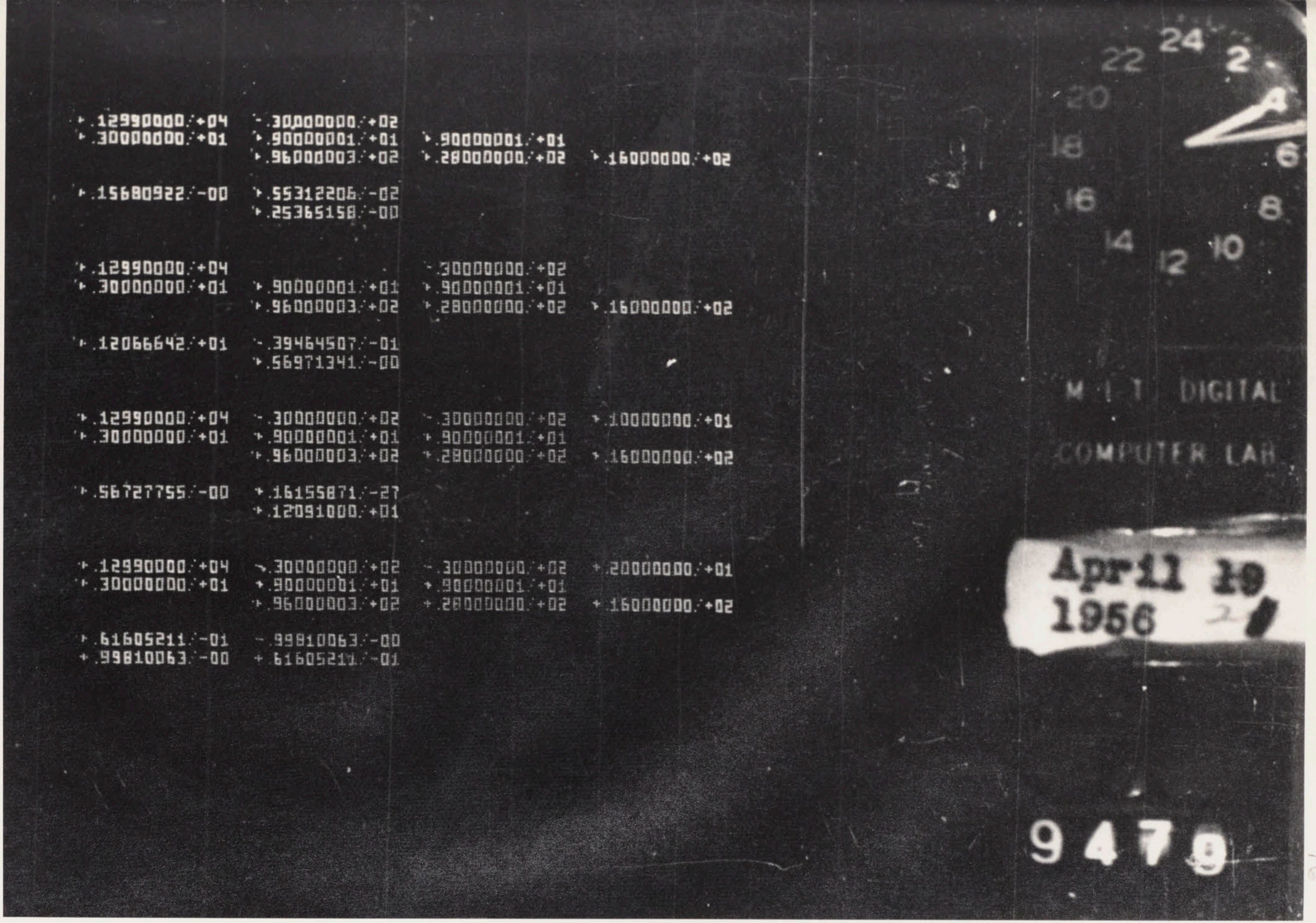


```
+.12990000/+04   -.30000000/+02
+.10000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.36000001/+02   +.12000000/+02

+.18307144/-00   +.13243580/-01
                 +.24502855/-00


+.12990000/+04                    -.30000000/+02
+.10000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.36000001/+02   +.12000000/+02

+.10606098/+01   -.94344734/-01
                 +.64199012/-00


+.12990000/+04   -.30000000/+02   -.30000000/+02   +.10000000/+01
+.10000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.36000001/+02   +.12000000/+02

+.62171006/-00   +.16155871/-27
                 +.10808899/+01


+.12990000/+04   -.30000000/+02   -.30000000/+02   +.20000000/+01
+.10000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.36000001/+02   +.12000000/+02

+.21015685/-00   -.97766768/-00
+.97766768/-00   +.21015685/-00
```

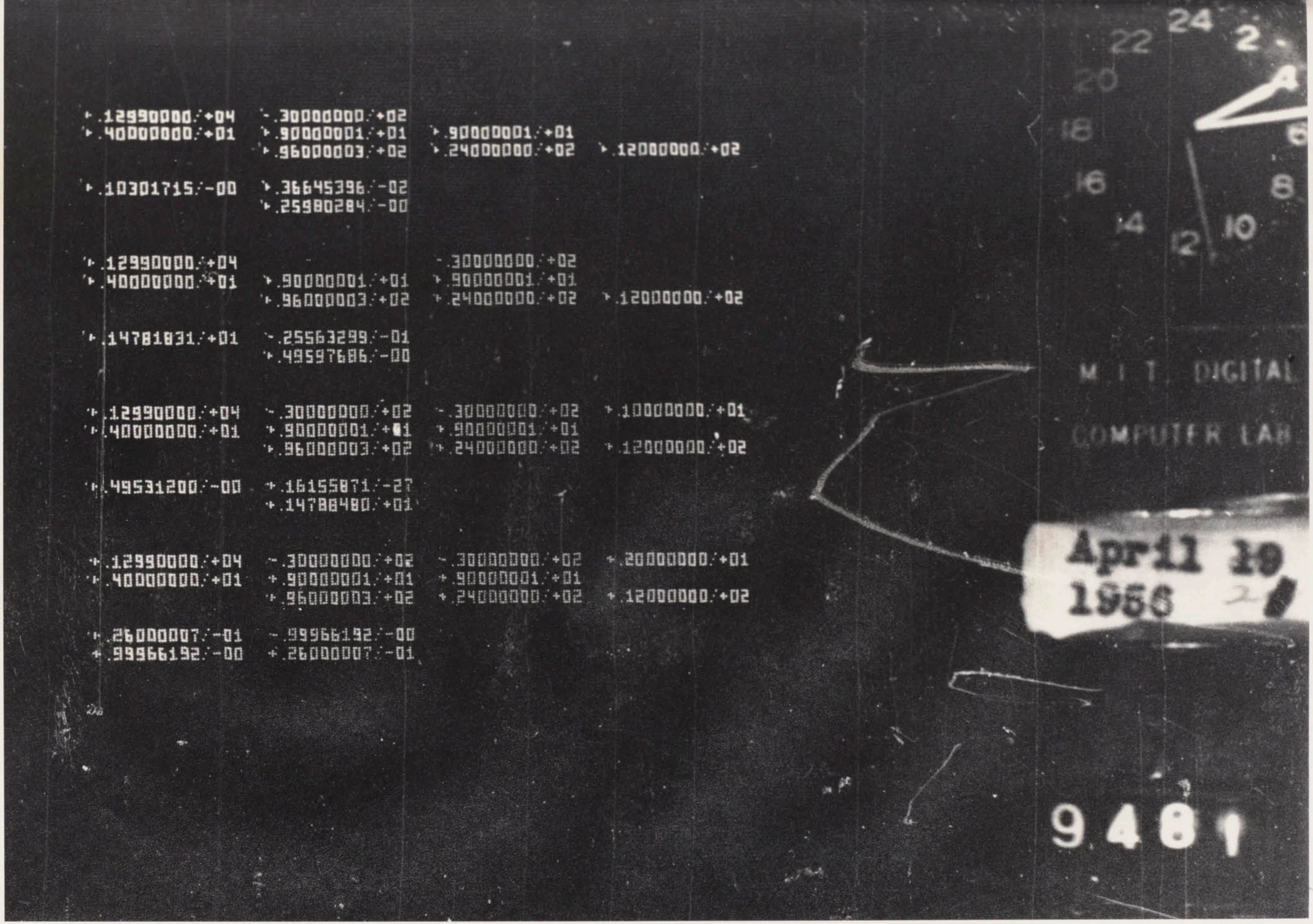


```
+.12990000./+04   -.30000000./+02
+.20000000./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.32000000./+02   +.20000000./+02

+.19454145./-00   +.79134814./-02
                  +.24393396./-00


+.12990000./+04                     -.30000000./+02
+.20000000./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.32000000./+02   +.20000000./+02

+.99746030./+00   -.56681007./-01
                  +.65940867./-00


+.12990000./+04   -.30000000./+02   -.30000000./+02   +.10000000./+01
+.20000000./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.32000000./+02   +.20000000./+02

+.65023607./-00   +.16155871./-27
                  +.10067129./+01


+.12990000./+04   -.30000000./+02   -.30000008./+02   +.20000000./+01
+.20000000./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.32000000./+02   +.20000000./+02

+.16110789./-00   -.98693680./-00
+.98693680./-00   +.16110789./-00
```

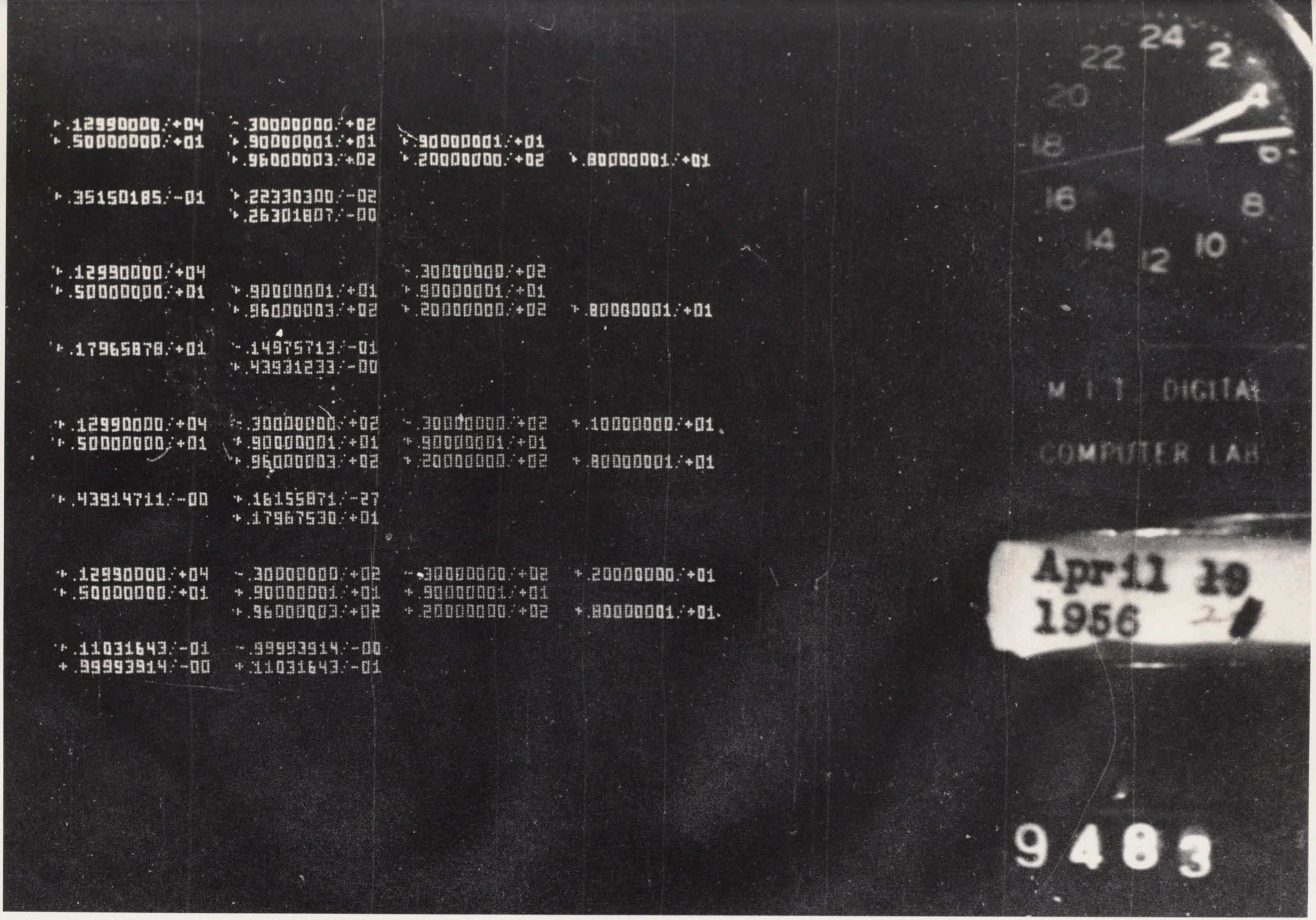
5



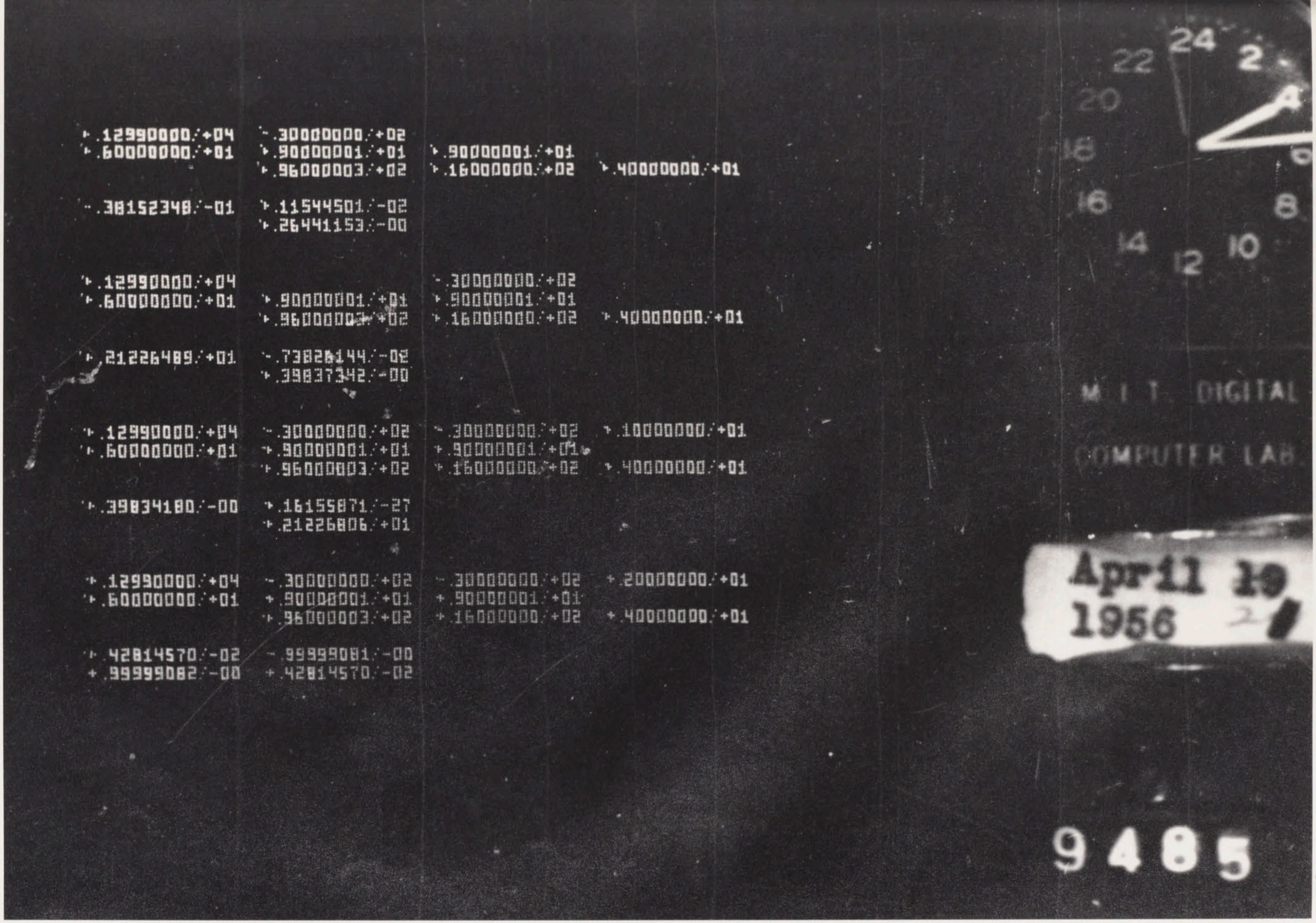
```
+.12990000./+04   -.30000000./+02
+.30000000./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.28000000./+02   +.16000000./+02

+.15680922./-00   +.55312206./-02
                  +.25365158./-00


+.12990000./+04                     -.30000000./+02
+.30000000./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.28000000./+02   +.16000000./+02

+.12066642./+01   -.39464507./-01
                  +.56971341./-00


+.12990000./+04   -.30000000./+02   -.30000000./+02   +.10000000./+01
+.30000000./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.28000000./+02   +.16000000./+02

+.56727755./-00   +.16155871./-27
                  +.12091000./+01


+.12990000./+04   -.30000000./+02   -.30000000./+02   +.20000000./+01
+.30000000./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.28000000./+02   +.16000000./+02

+.61605211./-01   -.99810063./-00
+.99810063./-00   +.61605211./-01
```



```
+.12990000./+04   -.30000000./+02
+.40000000./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.24000000./+02   +.12000000./+02

+.10301715./-00   +.36645396./-02
                  +.25980284./-00


+.12990000./+04                     -.30000000./+02
+.40000000./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.24000000./+02   +.12000000./+02

+.14781831./+01   -.25563299./-01
                  +.49597686./-00


+.12990000./+04   -.30000000./+02   -.30000000./+02   +.10000000./+01
+.40000000./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.24000000./+02   +.12000000./+02

+.49531200./-00   +.16155871./-27
                  +.14788480./+01


+.12990000./+04   -.30000000./+02   -.30000000./+02   +.20000000./+01
+.40000000./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.24000000./+02   +.12000000./+02

+.26000007./-01   -.99966192./-00
+.99966192./-00   +.26000007./-01
```



```
+.12990000.+04   -.30000000.+02
+.50000000.+01   +.90000001.+01   +.90000001.+01
                 +.96000003.+02   +.20000000.+02   +.80000001.+01

+.35150185.-01   +.22330300.-02
                 +.26301807.-00


+.12990000.+04                    -.30000000.+02
+.50000000.+01   +.90000001.+01   +.90000001.+01
                 +.96000003.+02   +.20000000.+02   +.80060001.+01

+.17965878.+01   -.14975713.-01
                 +.43931233.-00


+.12990000.+04   -.30000000.+02   -.30000000.+02   +.10000000.+01
+.50000000.+01   +.90000001.+01   +.90000001.+01
                 +.96000003.+02   +.20000000.+02   +.80000001.+01

+.43914711.-00   +.16155871.-27
                 +.17967530.+01


+.12990000.+04   -.30000000.+02   -.30000000.+02   +.20000000.+01
+.50000000.+01   +.90000001.+01   +.90000001.+01
                 +.96000003.+02   +.20000000.+02   +.80000001.+01

+.11031643.-01   -.99993914.-00
+.99993914.-00   +.11031643.-01
```



```
+.12990000/+04   -.30000000/+02
+.60000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.16000000/+02   +.40000000/+01

-.38152348/-01   +.11544501/-02
                 +.26441153/-00


+.12990000/+04                    -.30000000/+02
+.60000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.16000000/+02   +.40000000/+01

+.21226489/+01   -.73826144/-02
                 +.39837342/-00


+.12990000/+04   -.30000000/+02   -.30000000/+02   +.10000000/+01
+.60000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.16000000/+02   +.40000000/+01

+.39834180/-00   +.16155871/-27
                 +.21226806/+01


+.12990000/+04   -.30000000/+02   -.30000000/+02   +.20000000/+01
+.60000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.16000000/+02   +.40000000/+01

+.42814570/-02   -.99999081/-00
+.99999082/-00   +.42814570/-02
```

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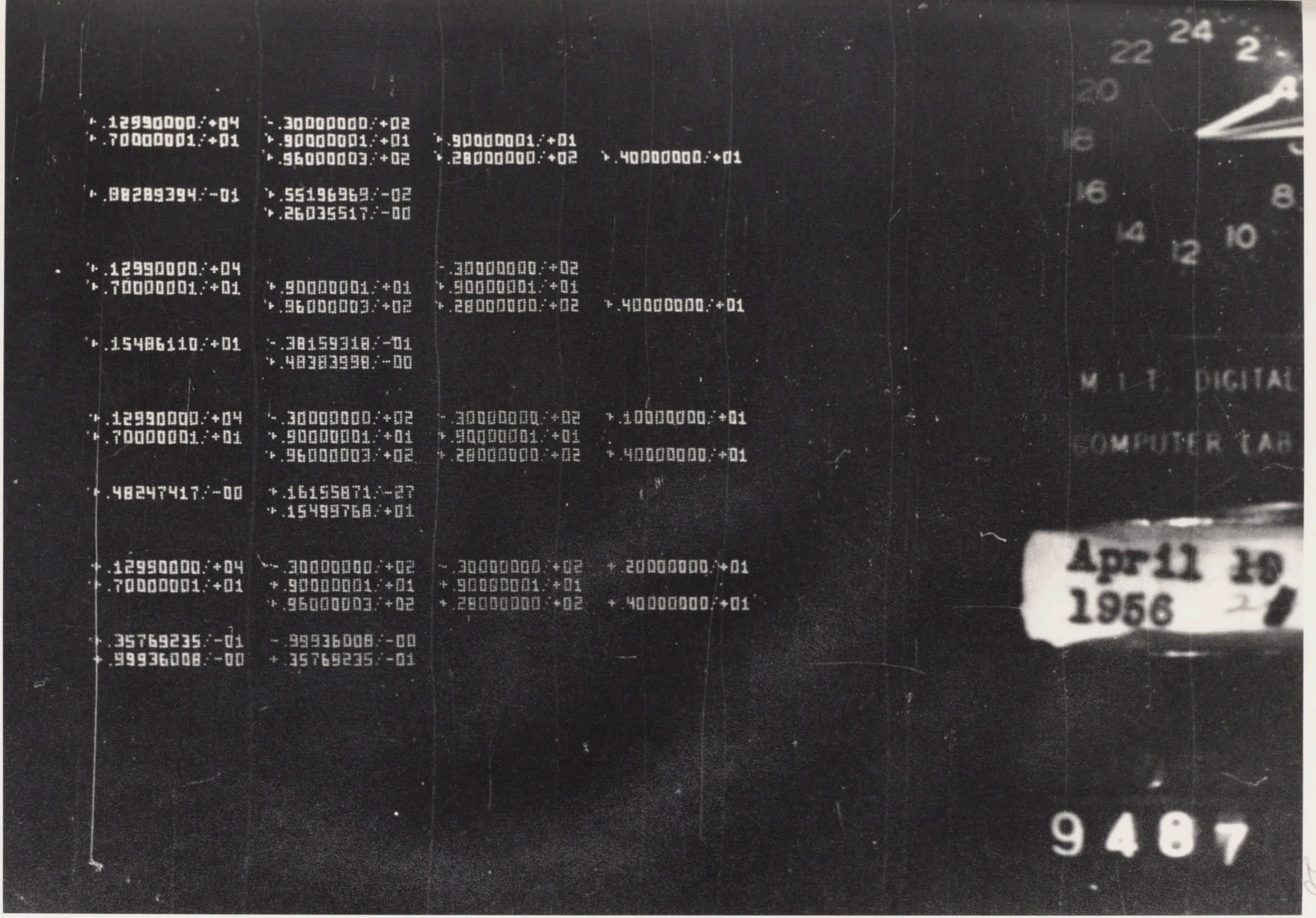
April 19
1956 2

9485



```
+.12990000./+04   -.30000000./+02
+.70000001./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.28000000./+02   +.40000000./+01

+.88289394./-01   +.55196969./-02
                  +.26035517./-00


+.12990000./+04                     -.30000000./+02
+.70000001./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.28000000./+02   +.40000000./+01

+.15486110./+01   -.38159318./-01
                  +.48383998./-00


+.12990000./+04   -.30000000./+02   -.30000000./+02   +.10000000./+01
+.70000001./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.28000000./+02   +.40000000./+01

+.48247417./-00   +.16155871./-27
                  +.15499768./+01


+.12990000./+04   -.30000000./+02   -.30000000./+02   +.20000000./+01
+.70000001./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.28000000./+02   +.40000000./+01

+.35769235./-01   -.99936008./-00
+.99936008./-00   +.35769235./-01
```

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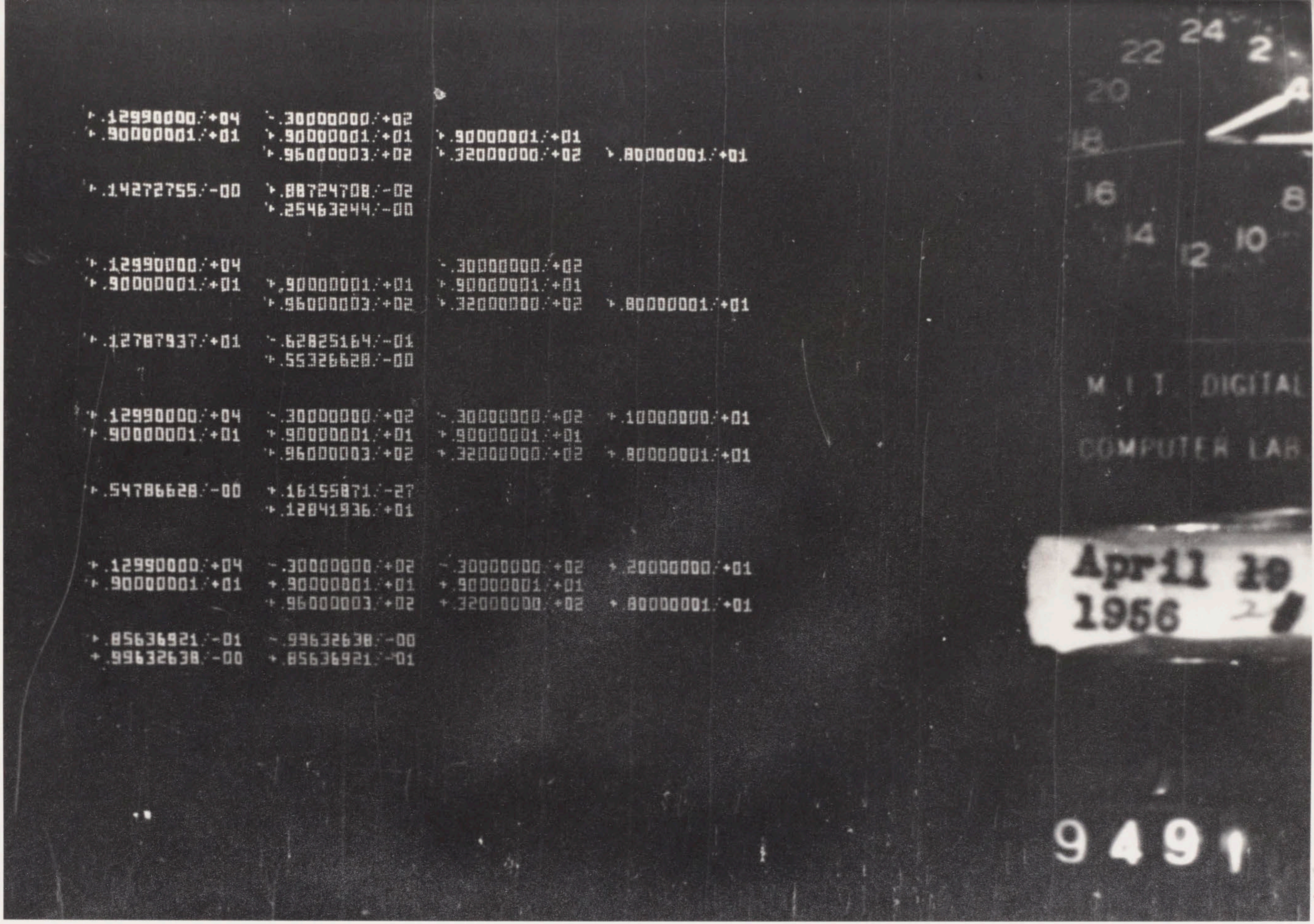
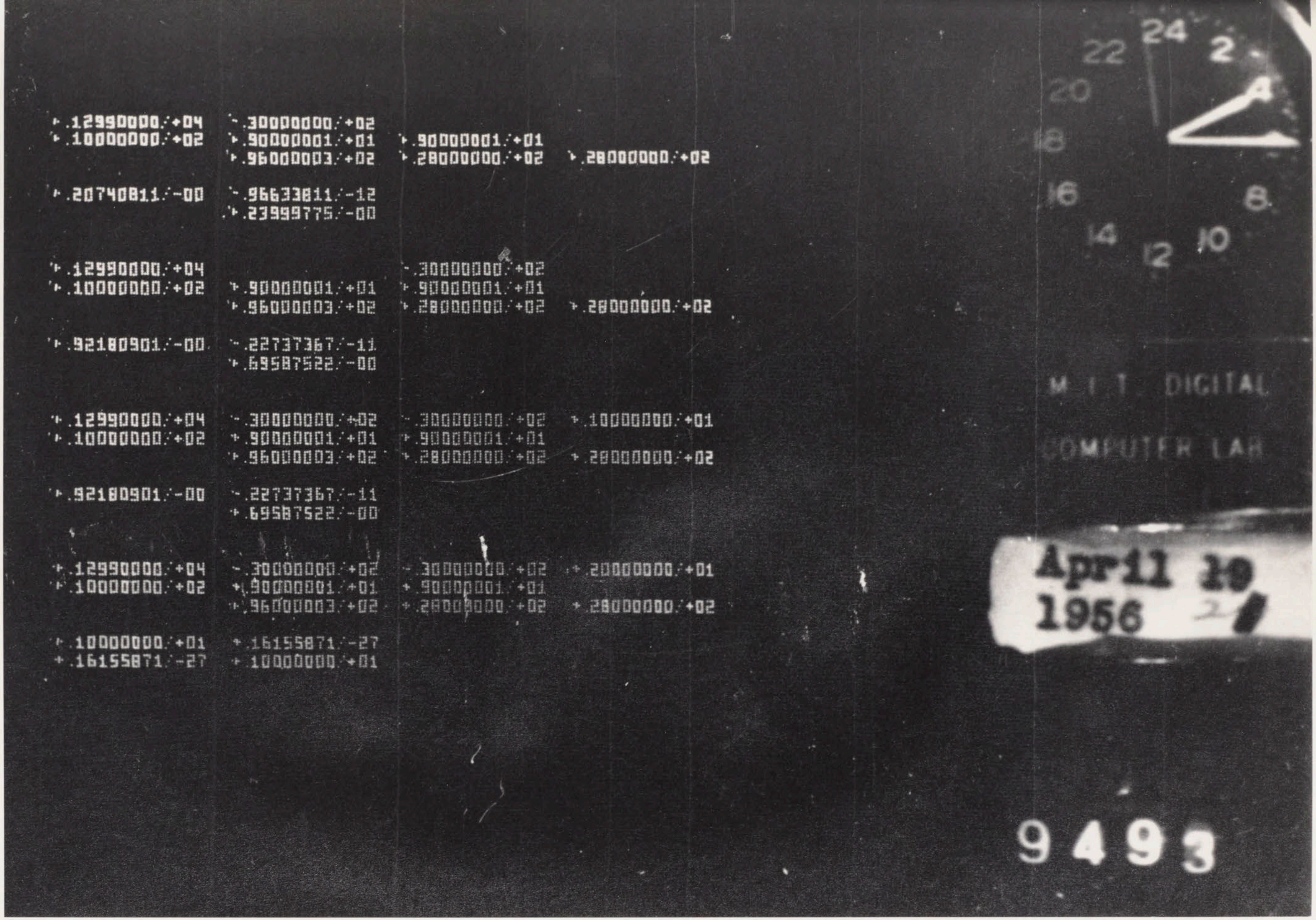
1956 2

9487



```
+.12990000./+04   -.30000000./+02
+.90000001./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.32000000./+02   +.80000001./+01

+.14272755./-00   +.88724708./-02
                  +.25463244./-00


+.12990000./+04                     -.30000000./+02
+.90000001./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.32000000./+02   +.80000001./+01

+.12787937./+01   -.62825164./-01
                  +.55326628./-00


+.12990000./+04   -.30000000./+02   -.30000000./+02   +.10000000./+01
+.90000001./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.32000000./+02   +.80000001./+01

+.54786628./-00   +.16155871./-27
                  +.12841936./+01


+.12990000./+04   -.30000000./+02   -.30000000./+02   +.20000000./+01
+.90000001./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.32000000./+02   +.80000001./+01

+.85636921./-01   -.99632638./-00
+.99632638./-00   +.85636921./-01
```



```
+.12990000./+04   -.30000000./+02
+.10000000./+02   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.28000000./+02   +.28000000./+02

+.20740811./-00   -.96633811./-12
                  +.23999775./-00


+.12990000./+04                     -.30000000./+02
+.10000000./+02   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.28000000./+02   +.28000000./+02

+.92180901./-00   -.22737367./-11
                  +.69587522./-00


+.12990000./+04   -.30000000./+02   -.30000000./+02   +.10000000./+01
+.10000000./+02   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.28000000./+02   +.28000000./+02

+.92180901./-00   -.22737367./-11
                  +.69587522./-00


+.12990000./+04   -.30000000./+02   -.30000000./+02   +.20000000./+01
+.10000000./+02   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.28000000./+02   +.28000000./+02

+.10000000./+01   +.16155871./-27
+.16155871./-27   +.10000000./+01
```

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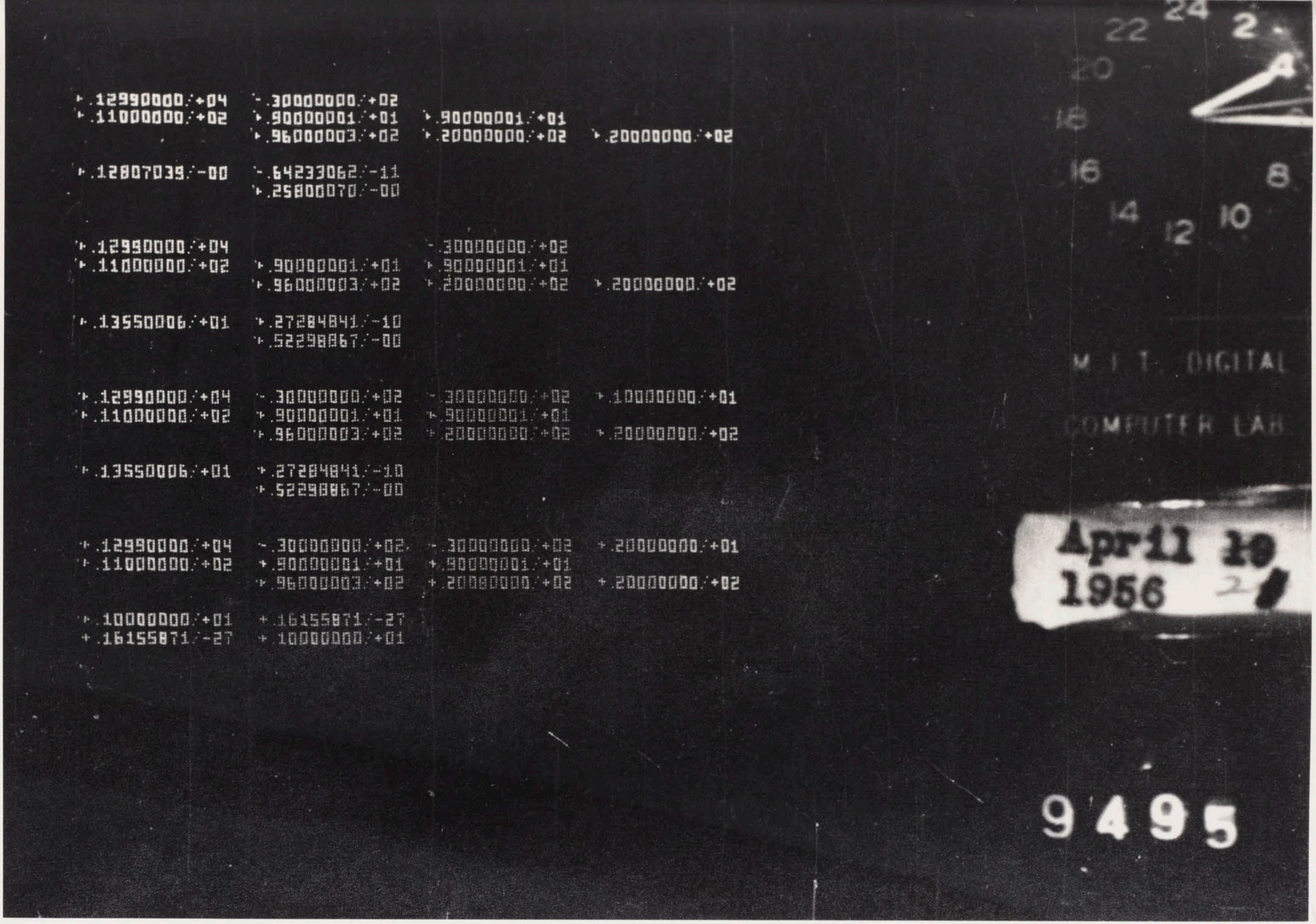
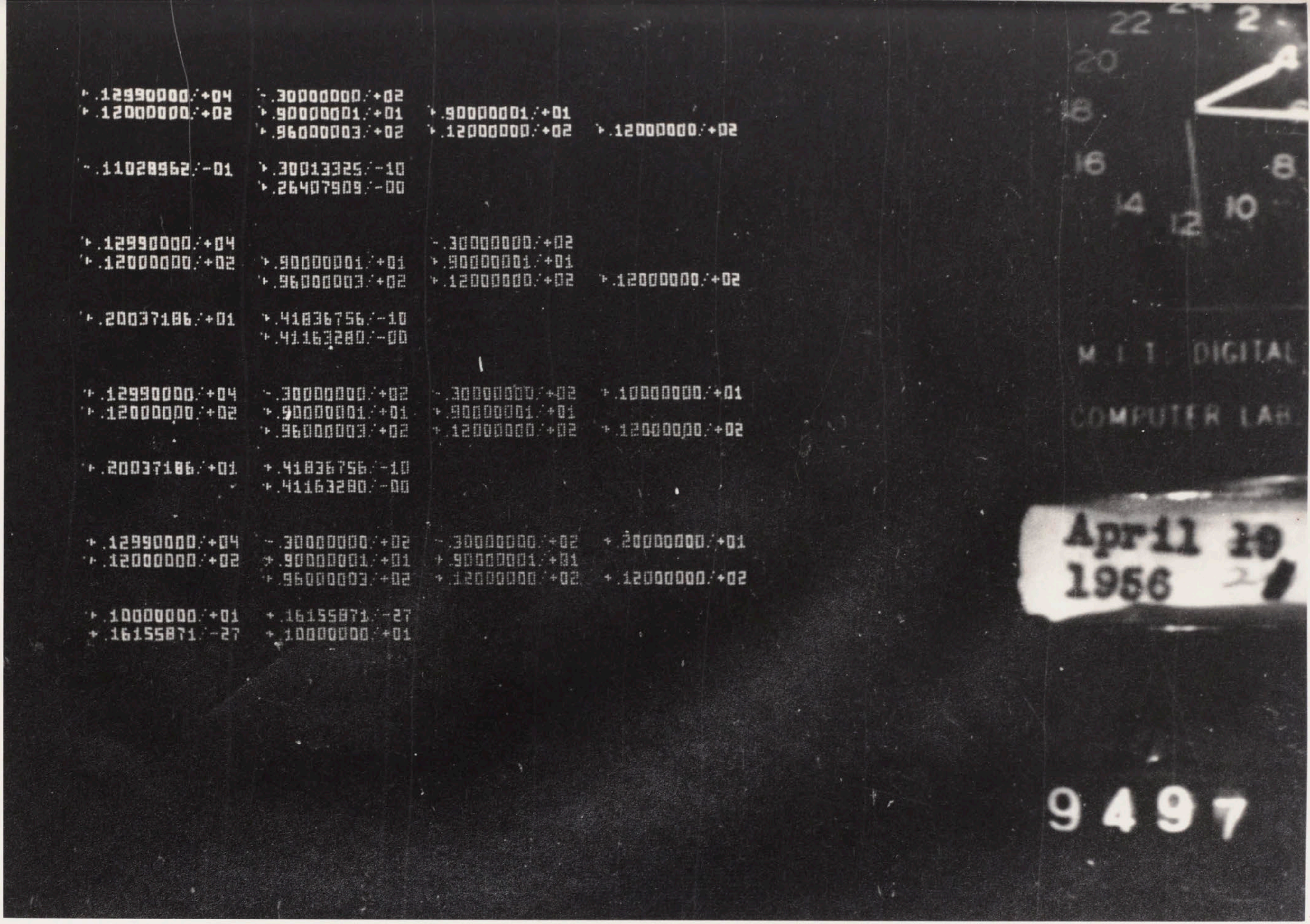
1956 2

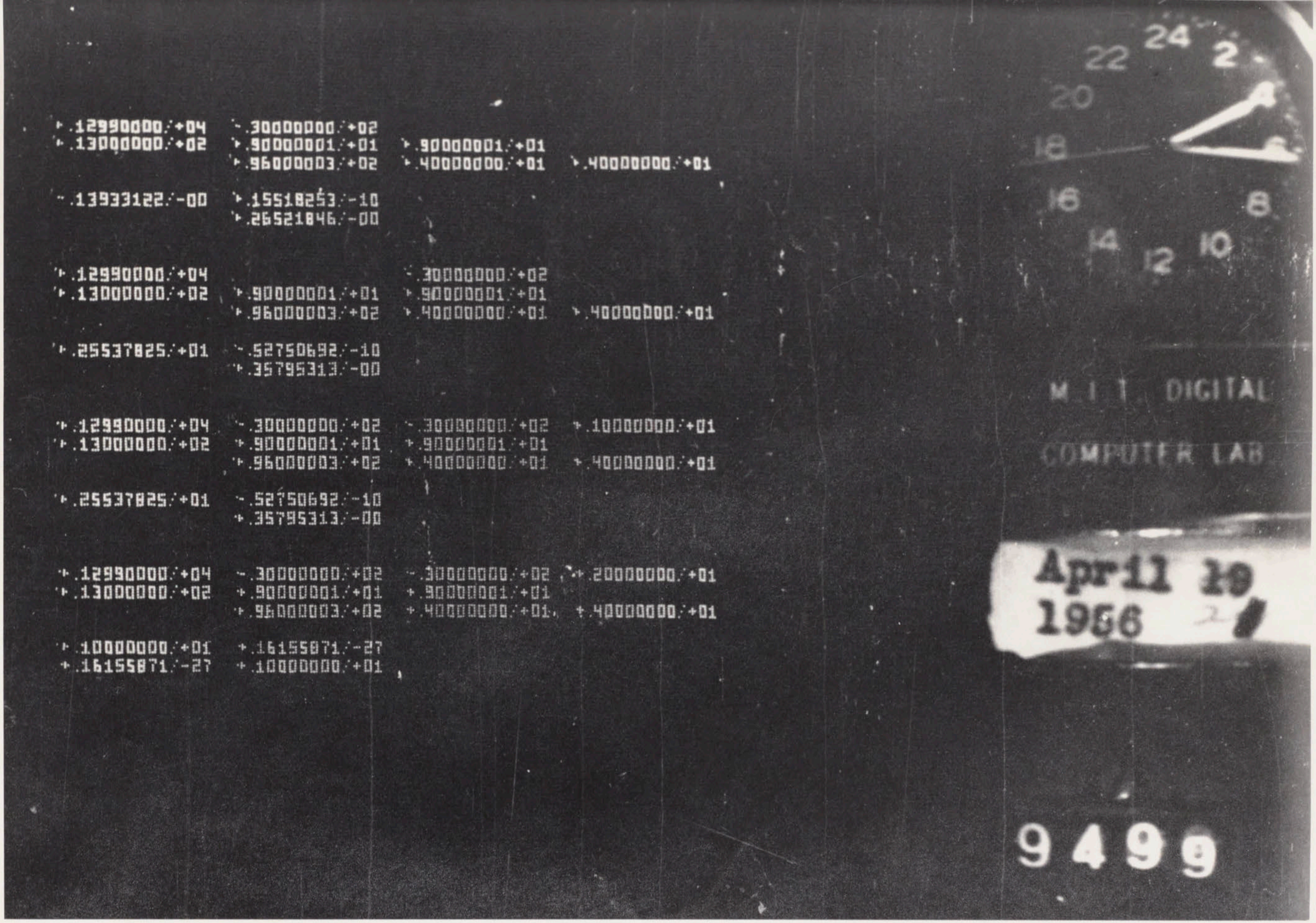
9493



```
+.12990000./+04   -.30000000./+02
+.11000000./+02   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.20000000./+02   +.20000000./+02

+.12807039./-00   -.64233062./-11
                  +.25800070./-00


+.12990000./+04                     -.30000000./+02
+.11000000./+02   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.20000000./+02   +.20000000./+02

+.13550006./+01   +.27284841./-10
                  +.52298867./-00


+.12990000./+04   -.30000000./+02   -.30000000./+02   +.10000000./+01
+.11000000./+02   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.20000000./+02   +.20000000./+02

+.13550006./+01   +.27284841./-10
                  +.52298867./-00


+.12990000./+04   -.30000000./+02   -.30000000./+02   +.20000000./+01
+.11000000./+02   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.20000000./+02   +.20000000./+02

+.10000000./+01   +.16155871./-27
+.16155871./-27   +.10000000./+01
```

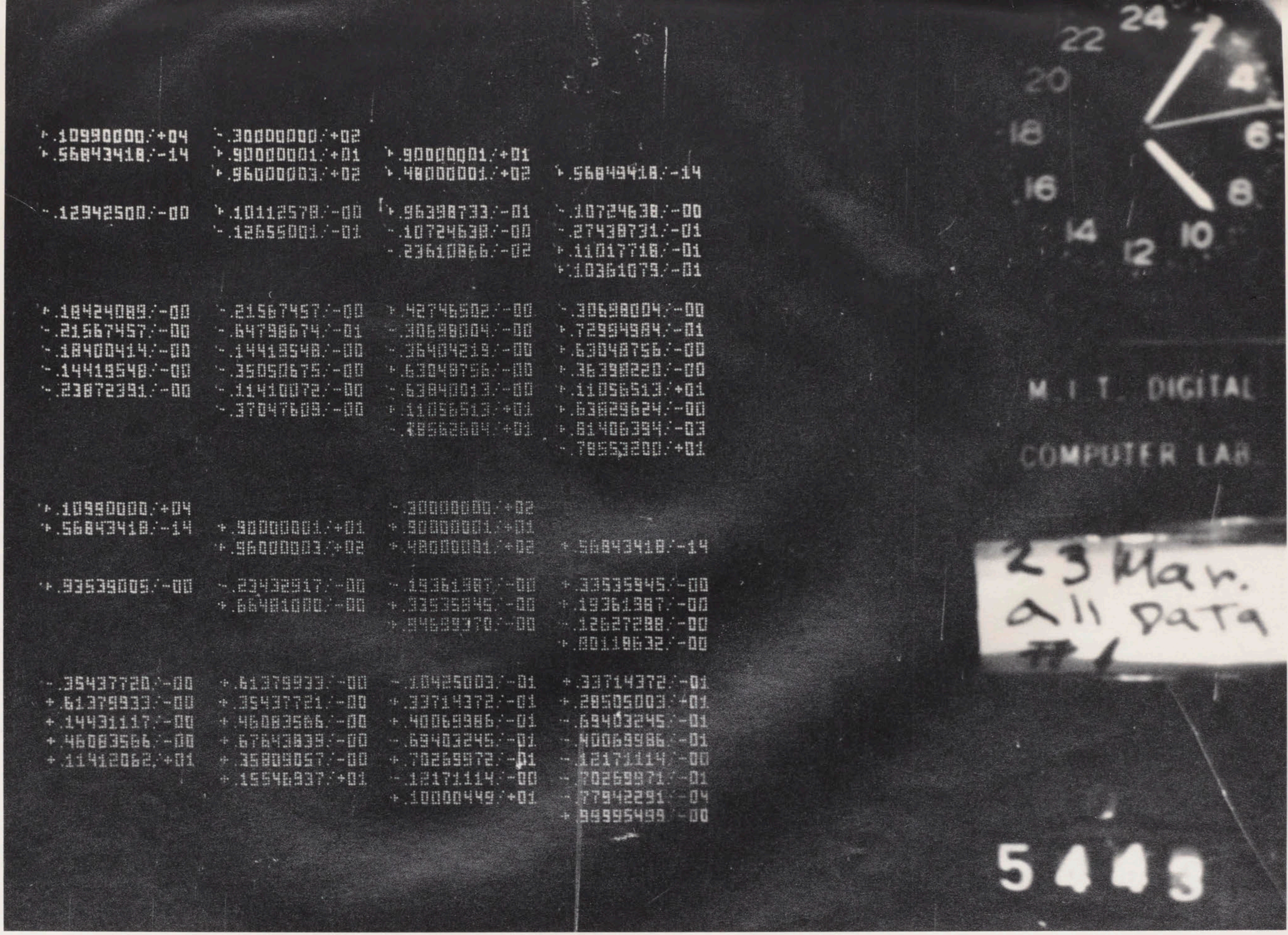


```
+.12990000./+04   -.30000000./+02
+.12000000./+02   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.12000000./+02   +.12000000./+02

-.11028962./-01   +.30013325./-10
                  +.26407909./-00


+.12990000./+04                     -.30000000./+02
+.12000000./+02   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.12000000./+02   +.12000000./+02

+.20037186./+01   +.41836756./-10
                  +.41163280./-00


+.12990000./+04   -.30000000./+02   -.30000000./+02   +.10000000./+01
+.12000000./+02   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.12000000./+02   +.12000000./+02

+.20037186./+01   +.41836756./-10
                  +.41163280./-00


+.12990000./+04   -.30000000./+02   -.30000000./+02   +.20000000./+01
+.12000000./+02   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.12000000./+02   +.12000000./+02

+.10000000./+01   +.16155871./-27
+.16155871./-27   +.10000000./+01
```



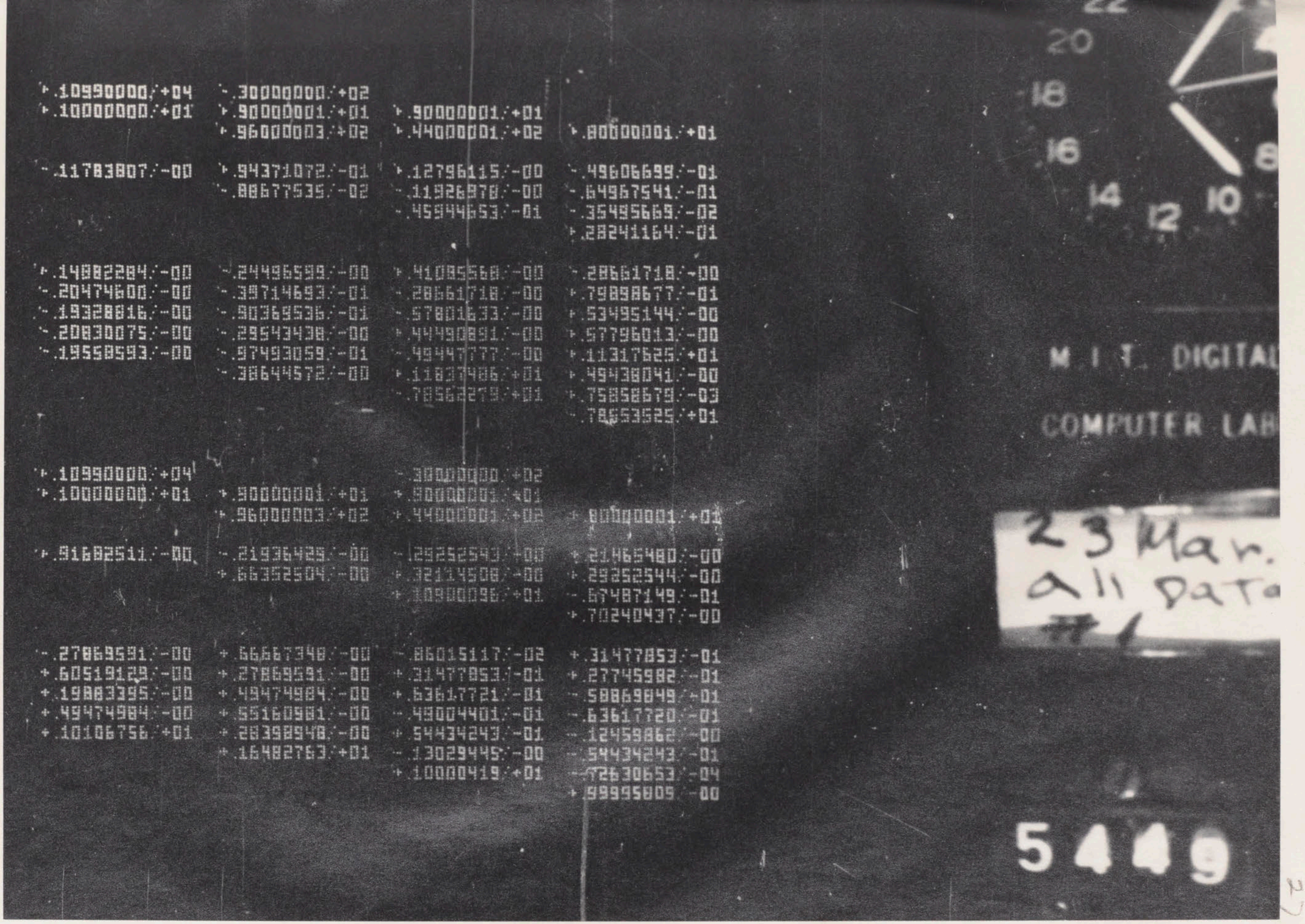
```
+.12990000./+04   -.30000000./+02
+.13000000./+02   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.40000000./+01   +.40000000./+01

-.13933122./-00   +.15518253./-10
                  +.26521846./-00


+.12990000./+04                     -.30000000./+02
+.13000000./+02   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.40000000./+01   +.40000000./+01

+.25537825./+01   -.52750692./-10
                  +.35795313./-00


+.12990000./+04   -.30000000./+02   -.30000000./+02   +.10000000./+01
+.13000000./+02   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.40000000./+01   +.40000000./+01

+.25537825./+01   -.52750692./-10
                  +.35795313./-00


+.12990000./+04   -.30000000./+02   -.30000000./+02   +.20000000./+01
+.13000000./+02   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.40000000./+01   +.40000000./+01

+.10000000./+01   +.16155871./-27
+.16155871./-27   +.10000000./+01
```

25



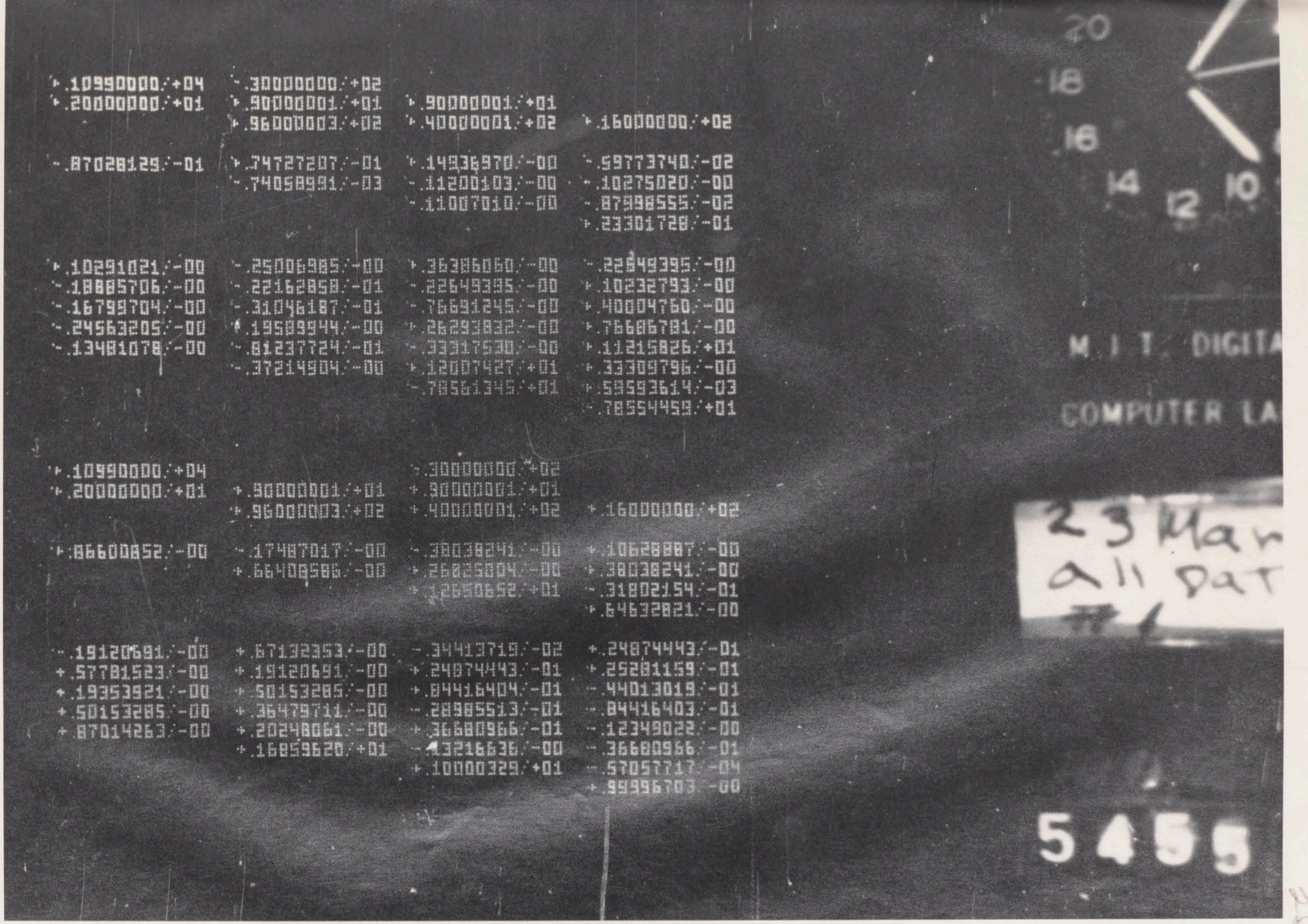
```
+.10990000./+04  -.30000000./+02
+.56843418./-14  +.90000001./+01  +.90000001./+01
                 +.96000003./+02  +.48000001./+02  +.56849418./-14

-.12942500./-00  +.10112578./-00  +.96398733./-01  -.10724638./-00
                 -.12655001./-01  -.10724638./-00  -.27438731./-01
                                  -.23610866./-02  +.11017718./-01
                                                   +.10361079./-01

+.18424089./-00  -.21567457./-00  +.42746502./-00  -.30698004./-00
-.21567457./-00  -.64798674./-01  -.30698004./-00  +.72954984./-01
-.18400414./-00  -.14419548./-00  -.36404219./-00  +.63048756./-00
-.14419548./-00  -.35050675./-00  +.63048756./-00  +.36398220./-00
-.23872391./-00  -.11410072./-00  -.63840013./-00  +.11056513./+01
                 -.37047609./-00  +.11056513./+01  +.63829624./-00
                                  -.78562604./+01  +.81406394./-03
                                                   -.78553200./+01


+.10990000./+04                   -.30000000./+02
+.56843418./-14  +.90000001./+01  +.90000001./+01
                 +.96000003./+02  +.48000001./+02  +.56843418./-14

+.93539005./-00  -.23432917./-00  -.19361987./-00  +.33535945./-00
                 +.66481000./-00  +.33535945./-00  +.19361987./-00
                                  +.94689370./-00  -.12627288./-00
                                                   +.00118632./-00

-.35437720./-00  +.61379933./-00  -.10425003./-01  +.33714372./-01
+.61379933./-00  +.35437721./-00  +.33714372./-01  +.28505003./-01
+.14431117./-00  +.46083566./-00  +.40069986./-01  -.69403245./-01
+.46083566./-00  +.67643839./-00  -.69403245./-01  -.40069986./-01
+.11412062./+01  +.35809057./-00  +.70269972./-01  -.12171114./-00
                 +.15546937./+01  -.12171114./-00  -.70269971./-01
                                  +.10000449./+01  -.77942291./-04
                                                   +.99995499./-00
```

23 Mar.
all Data
#1

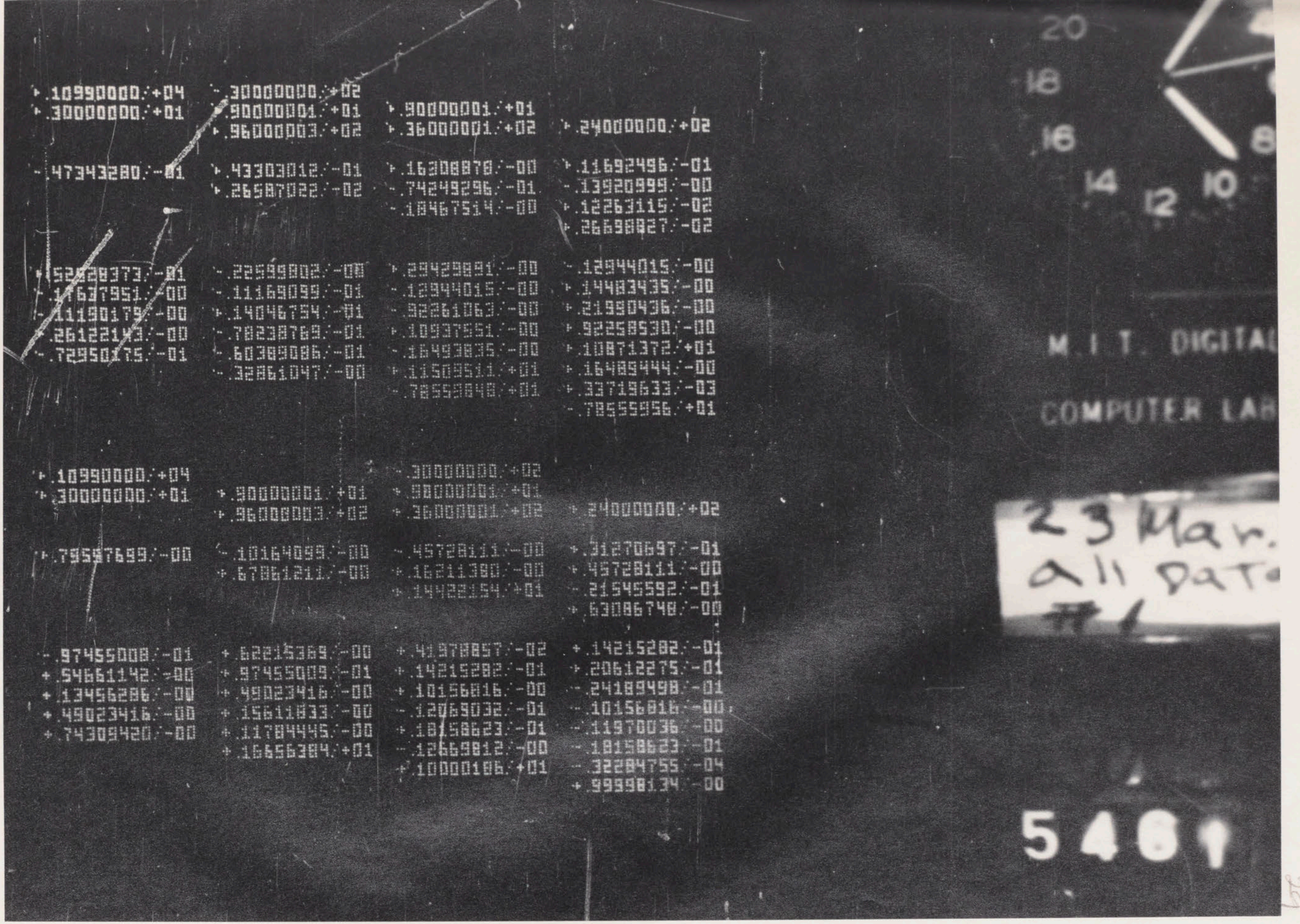


```
+.10990000/+04  -.30000000/+02
+.10000000/+01  +.90000001/+01  +.90000001/+01
                +.96000003/+02  +.44000001/+02  +.80000001/+01

-.11783807/-00  +.94371072/-01  +.12796115/-00  -.49606699/-01
                -.88677535/-02  -.11926978/-00  -.64967541/-01
                                -.45944653/-01  -.35495669/-02
                                                +.28241164/-01

+.14882284/-00  -.24496599/-00  +.41085568/-00  -.28661718/-00
-.20474600/-00  -.39714693/-01  -.28661718/-00  +.79898677/-01
-.19328816/-00  -.90369536/-01  -.57801633/-00  +.53495144/-00
-.20830075/-00  -.29543438/-00  +.44490891/-00  +.57796013/-00
-.19558593/-00  -.97493059/-01  -.49447777/-00  +.11317625/+01
                -.38644572/-00  +.11837486/+01  +.49438041/-00
                                -.78562279/+01  +.75858679/-03
                                                -.78653525/+01


+.10990000/+04                  -.30000000/+02
+.10000000/+01  +.90000001/+01  +.90000001/+01
                +.96000003/+02  +.44000001/+02  +.80000001/+01

+.91682511/-00  -.21936425/-00  -.29252543/-00  +.21465480/-00
                +.66352504/-00  +.32114508/-00  +.29252544/-00
                                +.10900096/+01  -.67487149/-01
                                                +.70240437/-00

-.27869591/-00  +.66667348/-00  -.86015117/-02  +.31477853/-01
+.60519129/-00  +.27869591/-00  +.31477853/-01  +.27745982/-01
+.19883395/-00  +.49474984/-00  +.63617721/-01  -.50869849/-01
+.49474984/-00  +.55160981/-00  -.49004401/-01  -.63617720/-01
+.10106756/+01  +.28398948/-00  +.54434243/-01  -.12459862/-00
                +.16482763/+01  -.13029445/-00  -.54434243/-01
                                +.10000419/+01  -.72630653/-04
                                                +.99995805/-00
```

23 Mar.
all Data
#1



```
+.10990000/+04  -.30000000/+02
+.20000000/+01  +.90000001/+01  +.90000001/+01
                +.96000003/+02  +.40000001/+02  +.16000000/+02

-.87028129/-01  +.74727207/-01  +.14936970/-00  -.59773740/-02
                -.74058991/-03  -.11200103/-00  -.10275020/-00
                                -.11007010/-00  -.87998555/-02
                                                +.23301728/-01

+.10291021/-00  -.25006985/-00  +.36386060/-00  -.22849395/-00
-.18885706/-00  -.22162858/-01  -.22649395/-00  +.10232793/-00
-.16799704/-00  -.31046187/-01  -.76691245/-00  +.40004760/-00
-.24563205/-00  +.19589944/-00  +.26293832/-00  +.76686781/-00
-.13481078/-00  -.81237724/-01  -.33317530/-00  +.11215826/+01
                -.37214904/-00  +.12007427/+01  +.33309796/-00
                                -.78561345/+01  +.59593614/-03
                                                -.78554459/+01


+.10990000/+04                  +.30000000/+02
+.20000000/+01  +.90000001/+01  +.90000001/+01
                +.96000003/+02  +.40000001/+02  +.16000000/+02

+.86600852/-00  -.17487017/-00  -.38038241/-00  +.10628887/-00
                +.66408586/-00  +.26025004/-00  +.38038241/-00
                                +.12650652/+01  -.31802154/-01
                                                +.64632821/-00

-.19120691/-00  +.67132353/-00  -.34413719/-02  +.24874443/-01
+.57781523/-00  +.19120691/-00  +.24874443/-01  +.25281159/-01
+.19353921/-00  +.50153285/-00  +.84416404/-01  -.44013019/-01
+.50153285/-00  +.36479711/-00  -.28985513/-01  -.84416403/-01
+.87014263/-00  +.20248061/-00  +.36680966/-01  -.12349022/-00
                +.16859620/+01  -.43216636/-00  -.36680966/-01
                                +.10000329/+01  -.57057717/-04
                                                +.99996703/-00
```

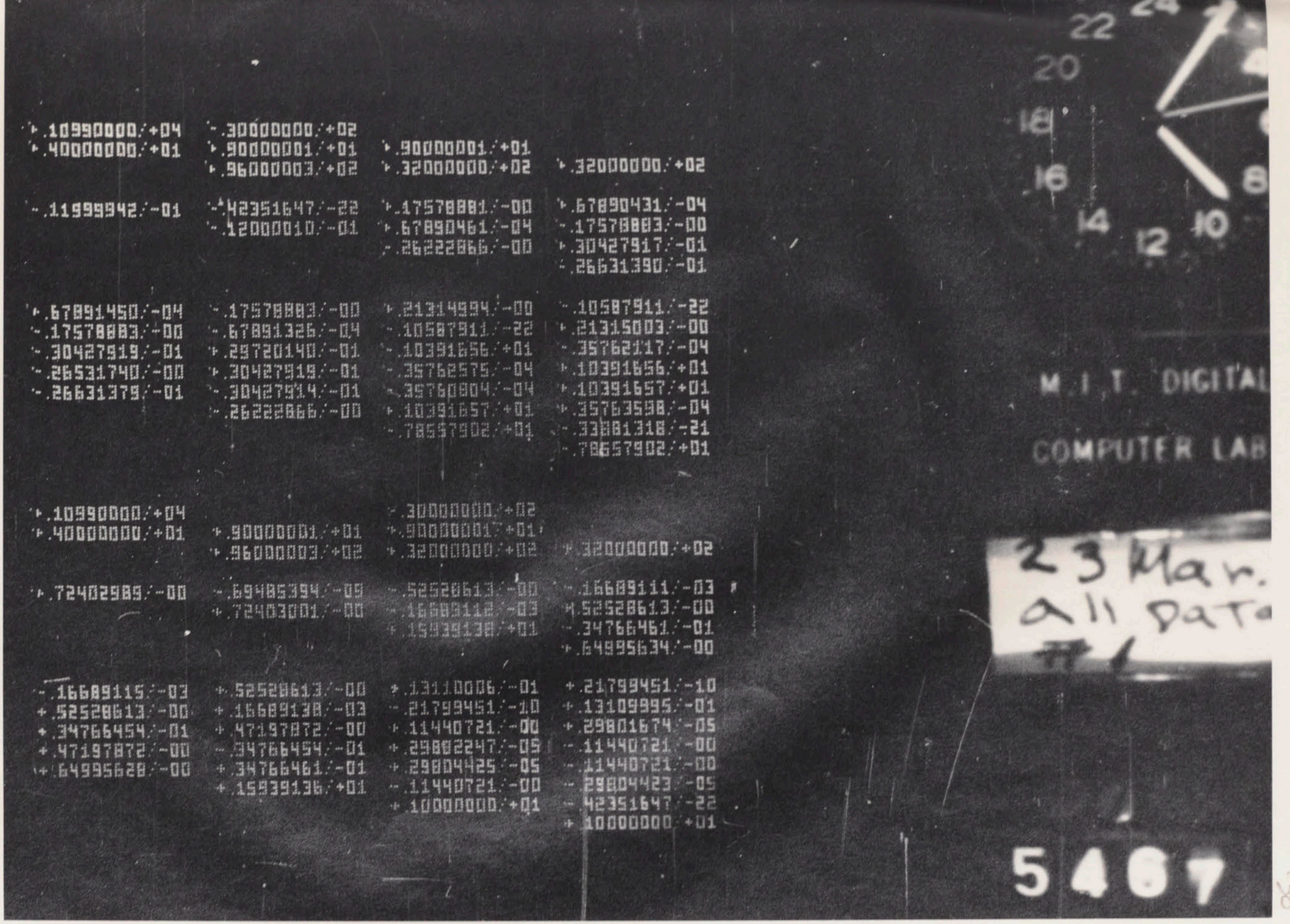


```
+.10990000:+04   -.30000000:+02
+.30000000:+01   +.90000001:+01   +.90000001:+01
                 +.96000003:+02   +.36000001:+02   +.24000000:+02

-.47343280:-01   +.43303012:-01   +.16308878:-00   +.11692496:-01
                 +.26587022:-02   -.74249296:-01   -.13920999:-00
                                  -.18467514:-00   +.12263115:-02
                                                   +.26698027:-02

+.52020373:-01   -.22599802:-00   +.29429891:-00   -.12944015:-00
+.17637951:-00   -.11169099:-01   -.12944015:-00   +.14403435:-00
-.11190179:-00   +.14046754:-01   -.92261063:-00   +.21990436:-00
+.26122143:-00   -.78238769:-01   +.10937551:-00   +.92258530:-00
-.72950175:-01   -.60309086:-01   -.16493835:-00   +.10871372:+01
                 -.32861047:-00   +.11509511:+01   +.16409444:-00
                                  -.78559848:+01   +.33719633:-03
                                                   -.78555956:+01


+.10990000:+04                    -.30000000:+02
+.30000000:+01   +.90000001:+01   +.90000001:+01
                 +.96000003:+02   +.36000001:+02   +.24000000:+02

+.79597699:-00   -.10164099:-00   -.45728111:-00   +.31270697:-01
                 +.67861211:-00   +.16211380:-00   +.45728111:-00
                                  +.14422154:+01   -.21545592:-01
                                                   +.63086748:-00

-.97455008:-01   +.62215369:-00   +.41978857:-02   +.14215282:-01
+.54661142:-00   +.97455009:-01   +.14215282:-01   +.20612275:-01
+.13456286:-00   +.49023416:-00   +.10156816:-00   -.24189498:-01
+.49023416:-00   +.15611833:-00   -.12069032:-01   -.10156816:-00
+.74309420:-00   +.11784445:-00   +.18158623:-01   -.11970036:-00
                 +.16656384:+01   -.12669812:-00   -.18158623:-01
                                  +.10000106:+01   -.32284755:-04
                                                   +.99998134:-00
```

M.I.T. DIGITA
COMPUTER LAB

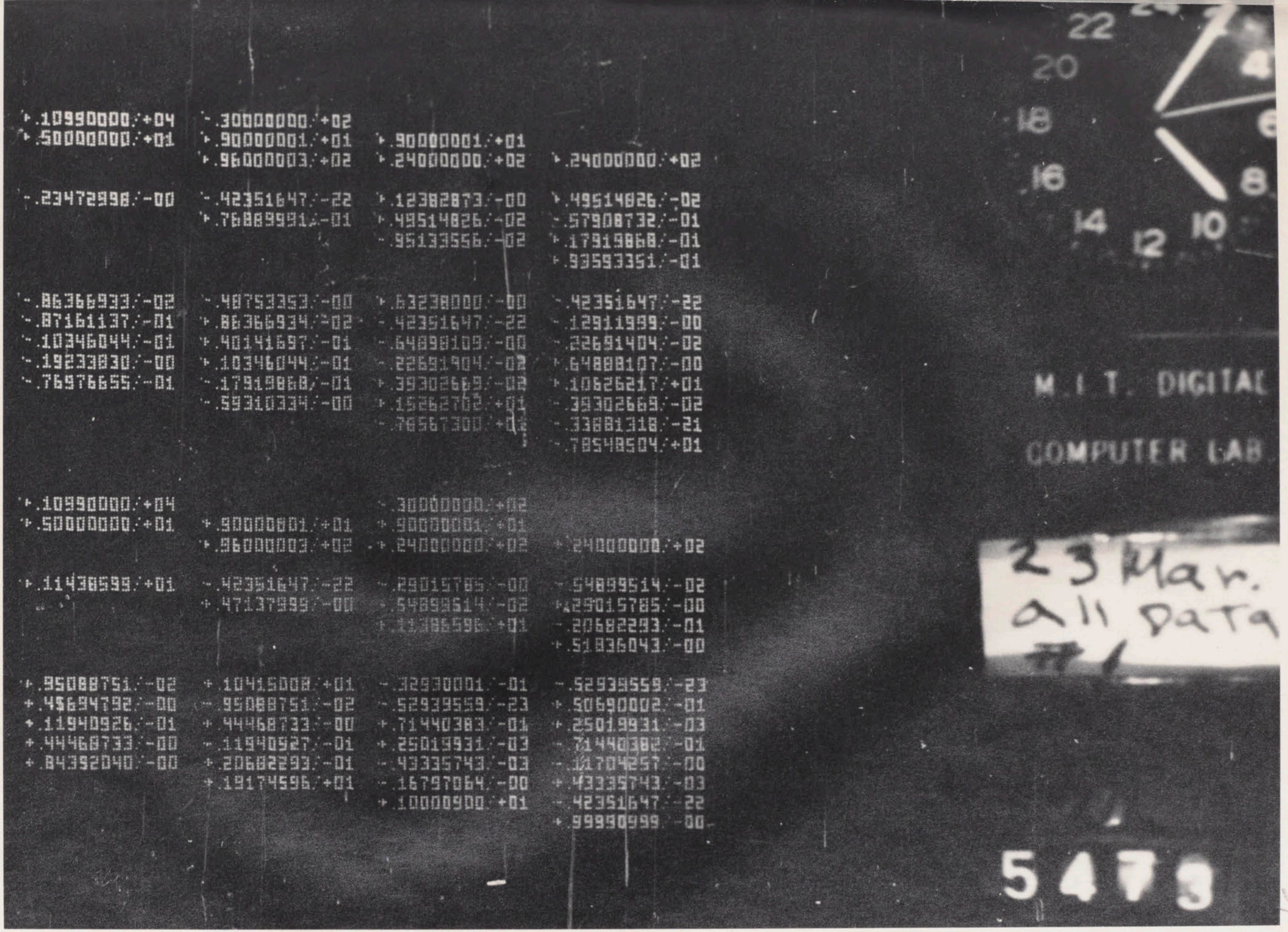
23 Mar.
all Data
#1

5461



```
+.10990000/+04   -.30000000/+02
+.40000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.32000000/+02   +.32000000/+02

-.11999942/-01   -.42351647/-22   +.17578881/-00   +.67890431/-04
                 -.12000010/-01   +.67890461/-04   -.17578803/-00
                                  -.26222866/-00   +.30427917/-01
                                                   -.26631390/-01

+.67891450/-04   -.17578803/-00   +.21314994/-00   -.10587911/-22
-.17578883/-00   -.67891326/-04   -.10587911/-22   +.21315003/-00
-.30427919/-01   +.29720140/-01   -.10391656/+01   -.35762117/-04
-.26531740/-00   +.30427919/-01   -.35762575/-04   +.10391656/+01
-.26631379/-01   -.30427914/-01   -.35760804/-04   +.10391657/+01
                 -.26222866/-00   +.10391657/+01   +.35763598/-04
                                  -.78557902/+01   -.33881318/-21
                                                   -.78657902/+01


+.10990000/+04                    -.30000000/+02
+.40000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.32000000/+02   +.32000000/+02

+.72402989/-00   -.69485394/-05   -.52528613/-00   -.16689111/-03
                 +.72403001/-00   -.16689112/-03   +.52528613/-00
                                  +.15939138/+01   -.34766461/-01
                                                   +.64995634/-00

-.16689115/-03   +.52528613/-00   +.13110006/-01   +.21799451/-10
+.52528613/-00   +.16689138/-03   -.21799451/-10   +.13109995/-01
+.34766454/-01   +.47197872/-00   +.11440721/-00   +.29801674/-05
+.47197872/-00   -.34766454/-01   +.29802247/-05   -.11440721/-00
+.64995628/-00   +.34766461/-01   +.29804425/-05   -.11440721/-00
                 +.15939136/+01   -.11440721/-00   -.29804423/-05
                                  +.10000000/+01   -.42351647/-22
                                                   +.10000000/+01
```

8

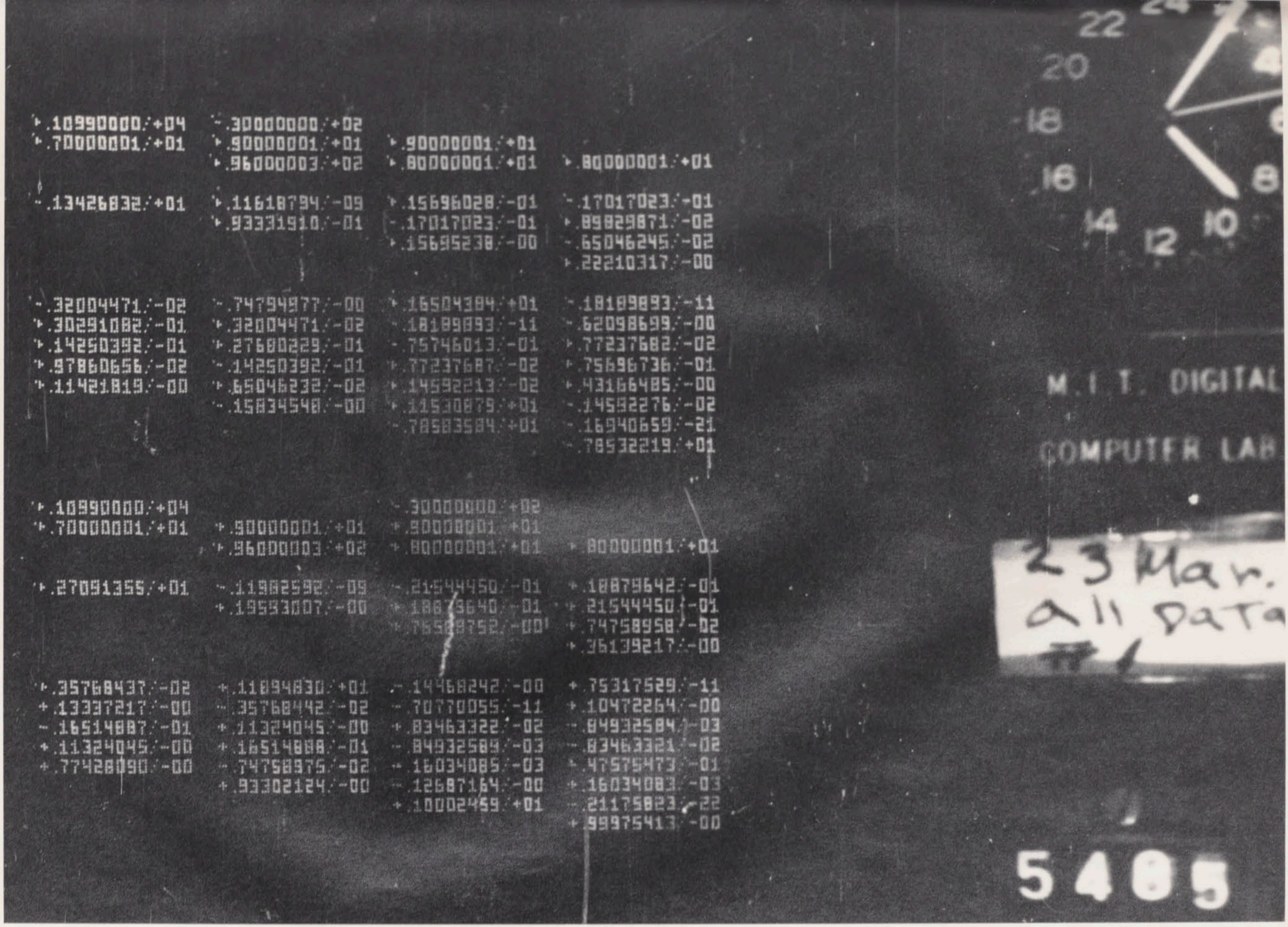


```
+.10990000/+04   -.30000000/+02
+.50000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.24000000/+02   +.24000000/+02

-.23472998/-00   -.42351647/-22   +.12382873/-00   +.49514826/-02
                 +.76889991/-01   +.49514826/-02   -.57908732/-01
                                  -.95133556/-02   +.17919868/-01
                                                   +.93593351/-01

-.86366933/-02   -.40753353/-00   +.63238000/-00   -.42351647/-22
-.87161137/-01   +.86366934/-02   -.42351647/-22   -.12911999/-00
-.10346044/-01   +.40141697/-01   -.64898109/-00   -.22691404/-02
-.19233030/-00   +.10346044/-01   -.22691904/-02   +.64888107/-00
-.76976655/-01   -.17919868/-01   +.39302669/-02   +.10626217/+01
                 -.59310334/-00   +.15262702/+01   -.39302669/-02
                                  -.76567300/+01   -.33881318/-21
                                                   -.78548504/+01


+.10990000/+04                    -.30000000/+02
+.50000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.24000000/+02   +.24000000/+02

+.11438599/+01   -.42351647/-22   -.29015785/-00   -.54899514/-02
                 +.47137999/-00   -.54899514/-02   +.29015785/-00
                                  +.11386596/+01   -.20682293/-01
                                                   +.51836043/-00

+.95088751/-02   +.10415008/+01   -.32930001/-01   -.52939559/-23
+.45694792/-00   -.95088751/-02   -.52939559/-23   +.50690002/-01
+.11940926/-01   +.44468733/-00   +.71440383/-01   +.25019931/-03
+.44468733/-00   -.11940927/-01   +.25019931/-03   -.71440382/-01
+.84392040/-00   +.20682293/-01   -.43335743/-03   -.11704257/-00
                 +.19174596/+01   -.16797064/-00   +.43335743/-03
                                  +.10000900/+01   -.42351647/-22
                                                   +.99990999/-00
```

23 Mar.
all Data
#1

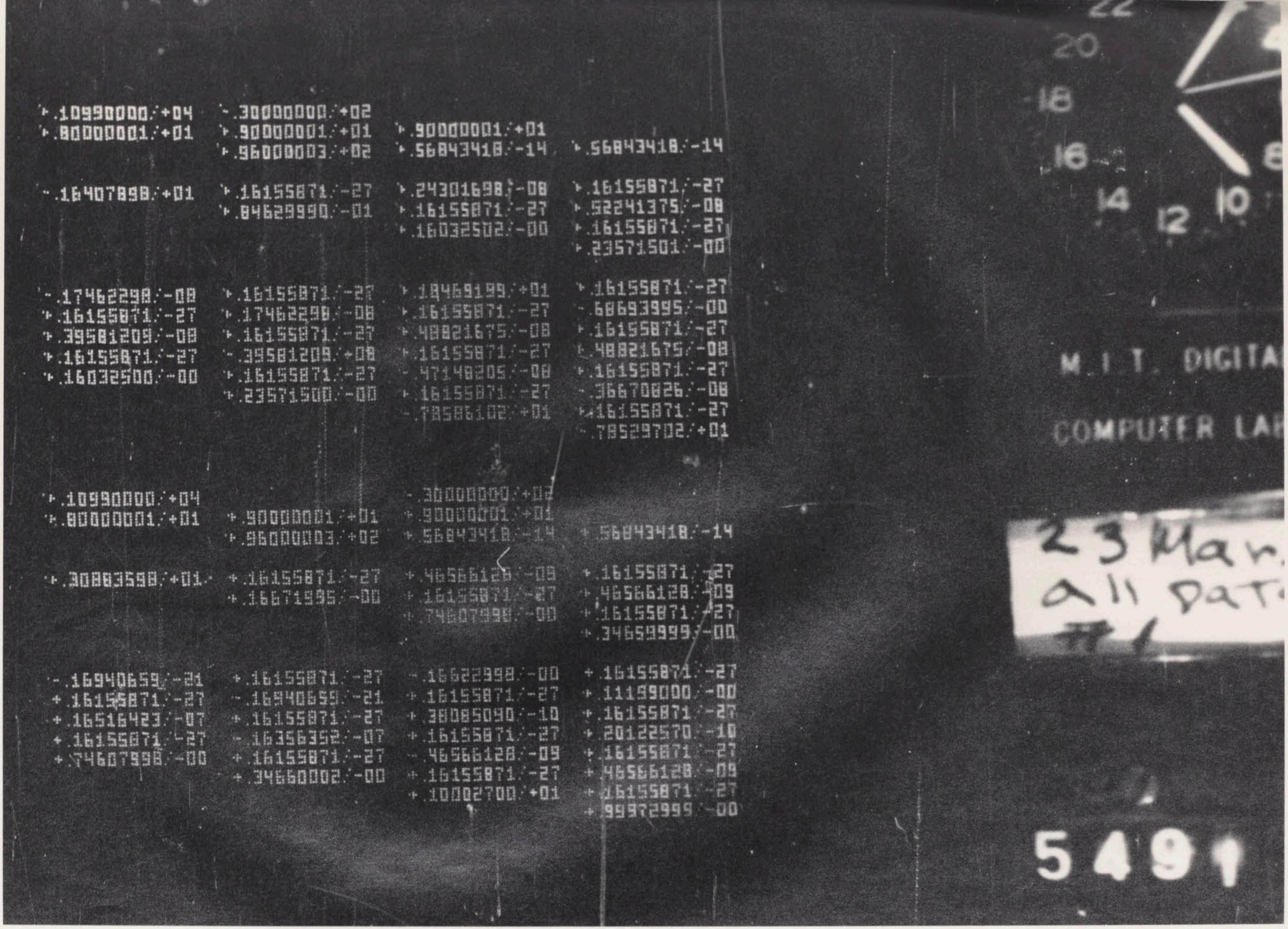
```
+.10990000/+04  -.30000000/+02
+.60000000/+01  +.90000001/+01  +.90000001/+01
                +.96000003/+02  +.16000000/+02  +.16000000/+02

-.72540001/-00  +.22737367/-12  +.61534546/-01  -.86593245/-02
                +.10363999/-00  -.86593245/+02  +.47854669/-02
                                +.11971069/-00  +.20340178/-03
                                                +.17610935/-00

-.87045858/-02  -.83691978/-00  +.11698900/+01  -.36379787/-11
+.40255463/-02  +.87045859/-02  -.36379787/-11  -.42751002/-00
+.20081873/-01  +.41576966/-01  -.30110260/-00  +.39421869/-02
-.66052681/-01  -.20081873/-01  +.39421878/-02  +.30098259/-00
+.24893227/-02  -.20340352/-03  +.39660283/-02  +.81545835/-00
                -.66082936/-00  +.16759412/+01  -.39660311/-02
                                -.78578704/+01  -.33881318/-21
                                                -.78539100/+01


+.10990000/+04                  -.30000000/+02
+.60000000/+01  +.90000001/+01  +.90000001/+01
                +.96000003/+02  +.16000000/+02  +.16000000/+02

+.10831501/+01  -.26579982/-09  -.11011428/-00  +.95645058/-02
                +.29154995/-00  +.95645058/-02  +.11011428/-00
                                +.86908662/-00  -.35210992/-03
                                                +.41830330/-00

+.96757663/-02  +.14664827/+01  -.91950013/-01  +.77591266/-11
+.28972730/-00  -.96757671/-02  +.60496319/-11  +.83450004/-01
-.22825525/-01  +.28387415/-00  +.33152233/-01  -.43435129/-03
+.28387415/-00  +.22825524/-01  -.43435135/-03  -.33152233/-01
+.84948337/-00  +.35210774/-03  -.43633789/-03  +.69858724/-01
                +.17808666/+01  -.18442870/-00  +.43633789/-03
                                +.10001800/+01  -.42351647/-22
                                                +.89981999/-00
```

23 Mar.
all Data
#1



```
+.10990000/+04   -.30000000/+02
+.70000001/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.80000001/+01   +.80000001/+01

-.13426832/+01   +.11618794/-09   +.15696028/-01   -.17017023/-01
                 +.93331910/-01   -.17017023/-01   +.89829871/-02
                                  +.15695238/-00   -.65046245/-02
                                                   +.22210317/-00

-.32004471/-02   -.74794977/-00   +.16504384/+01   -.18189893/-11
+.30291082/-01   +.32004471/-02   -.18189893/-11   -.62098699/-00
+.14250392/-01   +.27680229/-01   -.75746013/-01   +.77237682/-02
+.97860656/-02   -.14250392/-01   +.77237687/-02   +.75696736/-01
+.11421819/-00   +.65046232/-02   +.14592213/-02   +.43166485/-00
                 -.15834540/-00   +.11530879/+01   -.14592276/-02
                                  -.78583584/+01   -.16940659/-21
                                                   -.78532219/+01


+.10990000/+04                    -.30000000/+02
+.70000001/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.80000001/+01   +.80000001/+01

+.27091355/+01   -.11982592/-09   -.21544450/-01   +.18879642/-01
                 +.19553007/-00   +.18873640/-01   +.21544450/-01
                                  +.76588752/-00   +.74758958/-02
                                                   +.36139217/-00

+.35768437/-02   +.11094830/+01   -.14468242/-00   +.75317529/-11
+.13337217/-00   -.35768442/-02   -.70770055/-11   +.10472264/-00
-.16514887/-01   +.11324045/-00   +.83463322/-02   -.84932584/-03
+.11324045/-00   +.16514888/-01   -.84932589/-03   -.83463321/-02
+.77428090/-00   -.74758975/-02   -.16034085/-03   +.47575473/-01
                 +.93302124/-00   -.12687164/-00   +.16034083/-03
                                  +.10002459/+01   -.21175823/-22
                                                   +.99975413/-00
```

23 Mar.
all Data
#1



```
+.10990000./+04   -.30000000./+02
+.80000001./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.56843418./-14   +.56843418./-14

-.16407898./+01   +.16155871./-27   +.24301698./-08   +.16155871./-27
                  +.84629990./-01   +.16155871./-27   +.52241375./-08
                                    +.16032502./-00   +.16155871./-27
                                                      +.23571501./-00


-.17462298./-08   +.16155871./-27   +.18469199./+01   +.16155871./-27
+.16155871./-27   +.17462298./-08   +.16155871./-27   -.68693995./-00
+.39581209./-08   +.16155871./-27   +.48821675./-08   +.16155871./-27
+.16155871./-27   -.39581209./+08   +.16155871./-27   +.48821675./-08
+.16032500./-00   +.16155871./-27   -.47148205./-08   +.16155871./-27
                  +.23571500./-00   +.16155871./-27   -.36670826./-08
                                    -.78586102./+01   +.16155871./-27
                                                      -.78529702./+01


+.10990000./+04                     -.30000000./+02
+.80000001./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.56843418./-14   +.56843418./-14

+.30803598./+01   +.16155871./-27   +.46566128./-09   +.16155871./-27
                  +.16671995./-00   +.16155871./-27   +.46566128./-09
                                    +.74607998./-00   +.16155871./-27
                                                      +.34659999./-00


-.16940659./-21   +.16155871./-27   -.16622998./-00   +.16155871./-27
+.16155871./-27   -.16940659./-21   +.16155871./-27   +.11199000./-00
+.16516423./-07   +.16155871./-27   +.38085090./-10   +.16155871./-27
+.16155871./-27   -.16356352./-07   +.16155871./-27   +.20122570./-10
+.74607998./-00   +.16155871./-27   -.46566128./-09   +.16155871./-27
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                                    +.10002700./+01   +.16155871./-27
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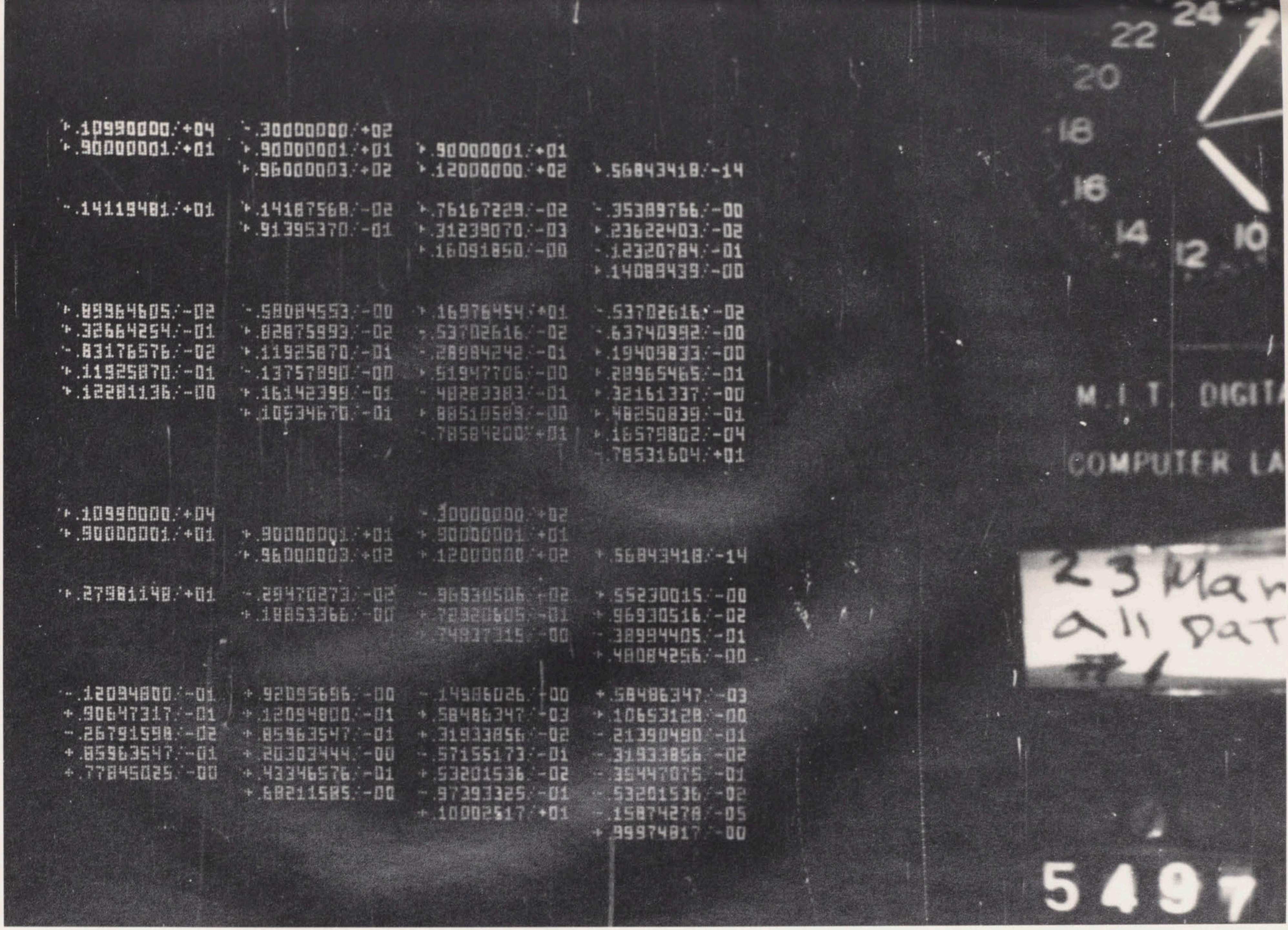

```
+.10990000. +04   -.30000000. +02
+.90000001. +01   +.90000001. +01   +.90000001. +01
                  +.96000003. +02   +.12000000. +02   +.56843418. -14

-.14119481. +01   +.14187568. -02   +.76167229. -02   -.35389766. -00
                  +.91395370. -01   +.31239070. -03   +.23622403. -02
                                    +.16091850. -00   -.12320784. -01
                                                      +.14089439. -00

+.89964605. -02   -.58084553. -00   +.16976454. +01   -.53702616. -02
+.32664254. -01   +.82875993. -02   -.53702616. -02   -.63740992. -00
-.83176576. -02   +.11925870. -01   -.28984242. -01   +.19409833. -00
+.11925870. -01   -.13757890. -00   +.51947706. -00   +.28965465. -01
+.12281136. -00   +.16142399. -01   -.48283383. -01   +.32161337. -00
                  +.10534670. -01   +.88510589. -00   +.48250839. -01
                                    -.78584200. +01   +.16579802. -04
                                                      -.78531604. +01


+.10990000. +04                     -.30000000. +02
+.90000001. +01   +.90000001. +01   +.90000001. +01
                  +.96000003. +02   +.12000000. +02   +.56843418. -14

+.27981148. +01   -.29470273. -02   -.96830506. +02   +.55230015. -00
                  +.18853366. -00   +.72920605. -01   +.96930516. -02
                                    +.74937315. -00   -.38994405. -01
                                                      +.48084256. -00

-.12094800. -01   +.92095696. -00   -.14986026. -00   +.58486347. -03
+.90647317. -01   +.12094800. -01   +.58486347. -03   +.10653128. -00
-.26791598. -02   +.85963547. -01   +.31933856. -02   -.21390490. -01
+.85963547. -01   +.20303444. -00   -.57155173. -01   -.31933856. -02
+.77845025. -00   +.43346576. -01   +.53201536. -02   -.39447075. -01
                  +.68211585. -00   -.97393325. -01   -.53201536. -02
                                    +.10002517. +01   -.15874278. -05
                                                      +.99974817. -00
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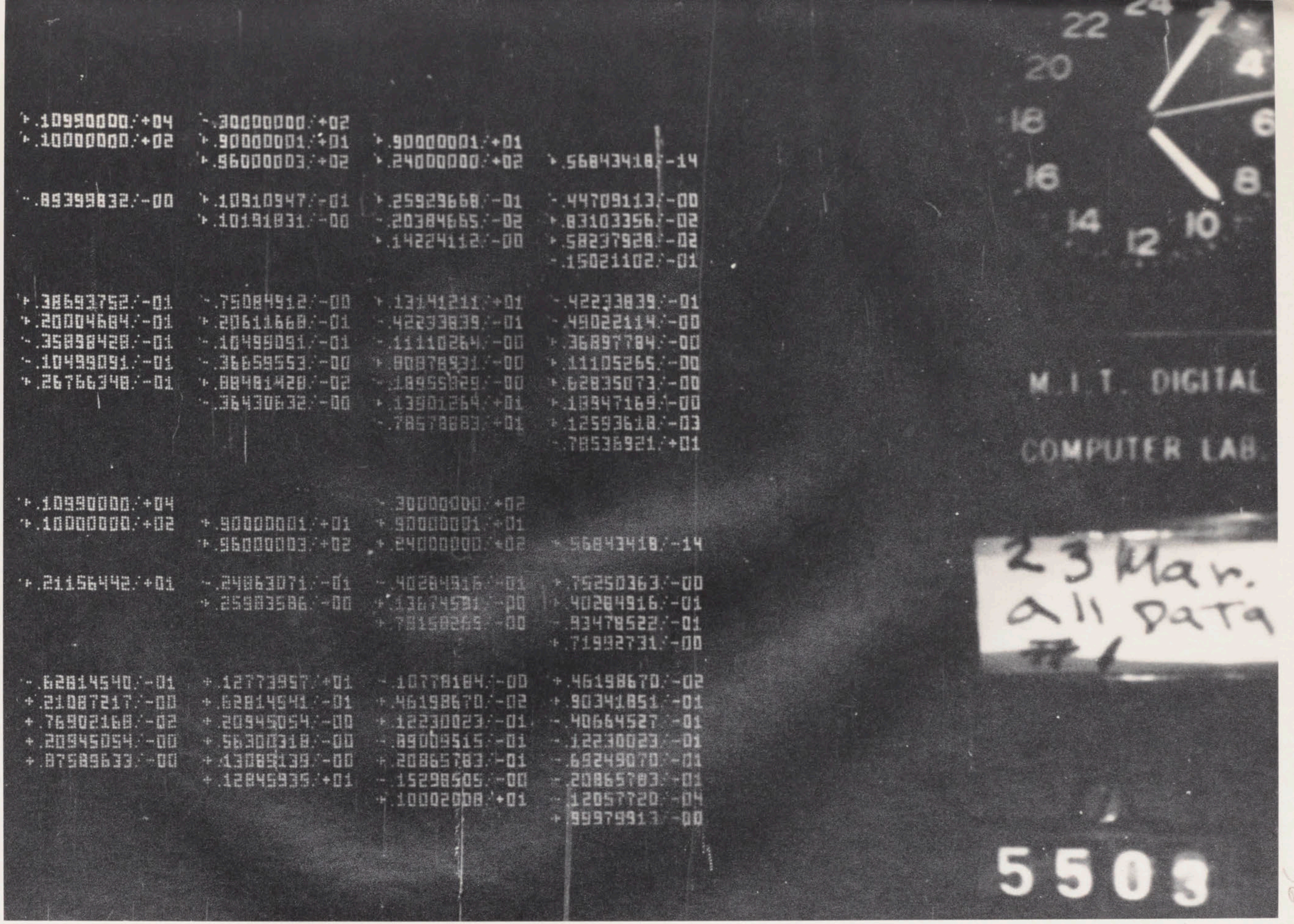

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+.10990000/+04     -.30000000/+02
+.10000000/+02     +.90000001/+01     +.90000001/+01
                   +.96000003/+02     +.24000000/+02     +.56843418/-14

-.89399832/-00     +.10910947/-01     +.25929668/-01     -.44709113/-00
                   +.10191831/-00     -.20384665/-02     +.83103356/-02
                                      +.14224112/-00     +.58237928/-02
                                                         -.15021102/-01

+.38693752/-01     -.75084912/-00     +.13141211/+01     -.42233839/-01
+.20004684/-01     +.20611668/-01     -.42233839/-01     -.49022114/-00
-.35898428/-01     -.10499091/-01     -.11110264/-00     +.36897784/-00
-.10499091/-01     -.36659553/-00     +.80878931/-00     +.11105265/-00
+.26766348/-01     +.88481428/-02     -.18955829/-00     +.62835073/-00
                   -.36430632/-00     +.13901264/+01     +.18947169/-00
                                      -.78578883/+01     +.12593618/-03
                                                         -.78536921/+01


+.10990000/+04                        -.30000000/+02
+.10000000/+02     +.90000001/+01     +.90000001/+01
                   +.96000003/+02     +.24000000/+02     +.56843418/-14

+.21156442/+01     -.24863071/-01     -.40284916/-01     +.75250363/-00
                   +.25983586/-00     +.13674591/-00     +.40284916/-01
                                      +.78150265/-00     -.93478522/-01
                                                         +.71992731/-00

-.62814540/-01     +.12773957/+01     -.10778184/-00     +.46198670/-02
+.21087217/-00     +.62814541/-01     +.46198670/-02     +.90341851/-01
+.76902168/-02     +.20945054/-00     +.12230023/-01     -.40664527/-01
+.20945054/-00     +.56300318/-00     -.89009515/-01     -.12230023/-01
+.87589633/-00     +.13089139/-00     +.20865783/-01     -.69249070/-01
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                                      +.10002008/+01     -.12057720/-04
                                                         +.99979913/-00
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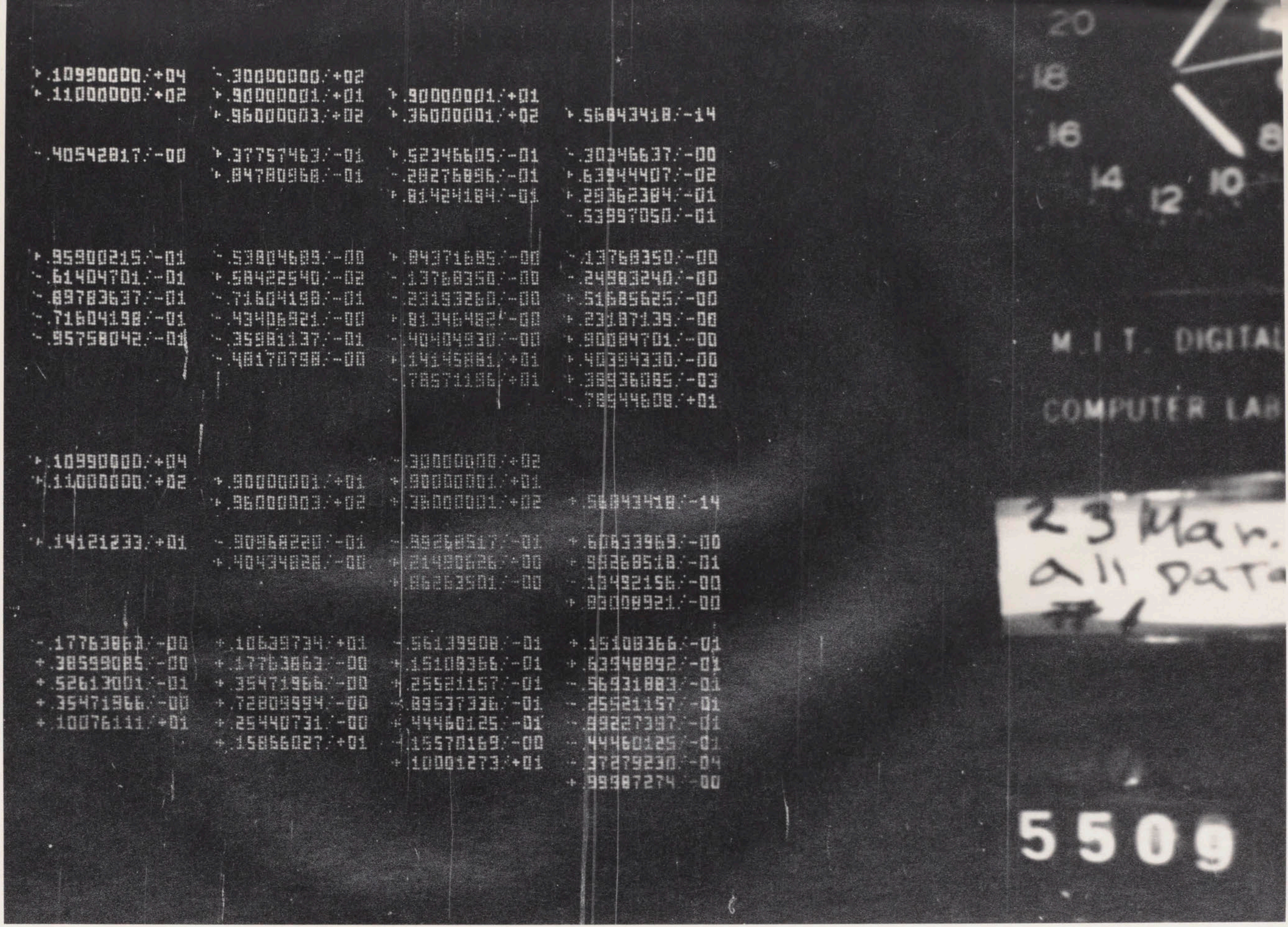

```
+.10990000:+04  -.30000000:+02
+.11000000:+02  +.90000001:+01  +.90000001:+01
                +.96000003:+02  +.36000001:+02  +.56043418:-14

-.40542817:-00  +.37757463:-01  +.52346605:-01  -.30346637:-00
                +.84780960:-01  -.28276896:-01  +.63944407:-02
                                +.81424184:-01  +.29362384:-01
                                                -.53997050:-01

+.95900215:-01  -.53804609:-00  +.84371685:-00  -.13760350:-00
-.61404701:-01  +.58422540:-02  -.13760350:-00  -.24983240:-00
-.89783637:-01  -.71604198:-01  -.23193260:-00  +.51685625:-00
-.71604198:-01  -.43406921:-00  +.81346482:-00  +.23187139:-00
-.95758042:-01  -.35981137:-01  -.40404930:-00  +.90084701:-00
                -.48170798:-00  +.14145881:+01  +.40394330:-00
                                -.78571196:+01  +.38936085:-03
                                                -.78944608:+01


+.10990000:+04                  -.30000000:+02
+.11000000:+02  +.90000001:+01  +.90000001:+01
                +.96000003:+02  +.36000001:+02  +.56043418:-14

+.14121233:+01  -.90968220:-01  -.89260517:-01  +.60633969:-00
                +.40434028:-00  +.21490626:-00  +.98268518:-01
                                +.86263501:-00  -.18492156:-00
                                                +.80008921:-00

-.17763863:-00  +.10639734:+01  -.56139908:-01  +.15108366:-01
+.38599085:-00  +.17763863:-00  +.15108366:-01  +.63948892:-01
+.52613001:-01  +.35471966:-00  +.25521157:-01  -.56931883:-01
+.35471966:-00  +.72809994:-00  -.89537336:-01  -.25521157:-01
+.10076111:+01  +.25440731:-00  +.44460125:-01  -.89227397:-01
                +.15866027:+01  -.15570169:-00  -.44460125:-01
                                +.10001273:+01  +.37279230:-04
                                                +.99987274:-00
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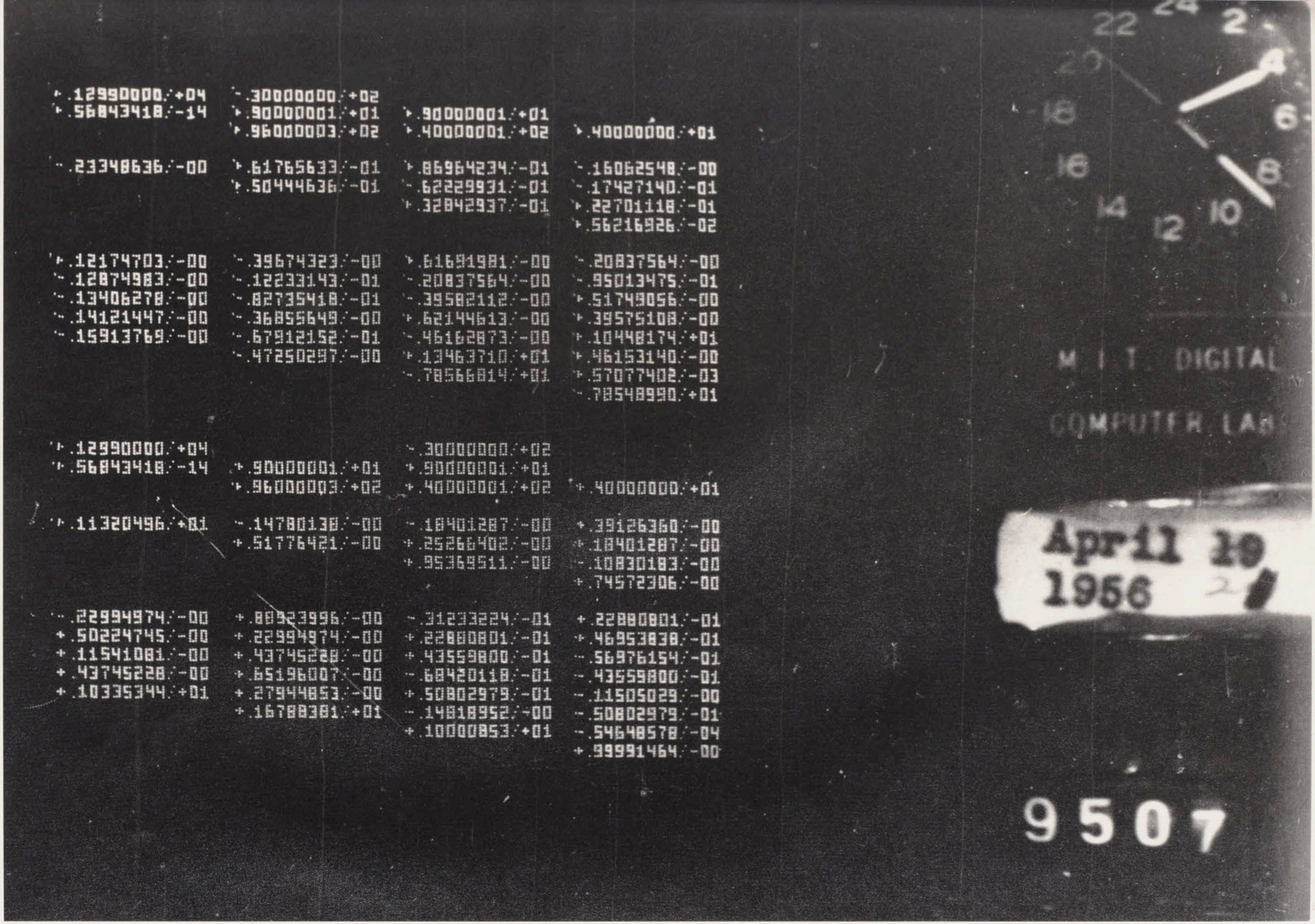

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+.12990000./+04  -.30000000./+02
+.56843418./-14  +.90000001./+01  +.90000001./+01
                 +.96000003./+02  +.40000001./+02  +.40000000./+01

-.23348636./-00  +.61765633./-01  +.86964234./-01  -.16062548./-00
                 +.50444636./-01  -.62229931./-01  -.17427140./-01
                                  +.32842937./-01  +.22701118./-01
                                                   +.56216926./-02

+.12174703./-00  -.39674323./-00  +.61691981./-00  -.20837564./-00
-.12874983./-00  -.12233143./-01  -.20837564./-00  -.95013475./-01
-.13406278./-00  -.82735418./-01  -.39582112./-00  +.51749056./-00
-.14121447./-00  -.36855649./-00  +.62144613./-00  +.39575108./-00
-.15913769./-00  -.67912152./-01  -.46162873./-00  +.10448174./+01
                 -.47250297./-00  +.13463710./+01  +.46153140./-00
                                  -.78566814./+01  +.57077402./-03
                                                   -.78548990./+01


+.12990000./+04                   -.30000000./+02
+.56843418./-14  +.90000001./+01  +.90000001./+01
                 +.96000003./+02  +.40000001./+02  +.40000000./+01

+.11320496./+01  -.14780138./-00  -.18401287./-00  +.39126360./-00
                 +.51776421./-00  +.25266402./-00  +.18401287./-00
                                  +.95369511./-00  -.10830183./-00
                                                   +.74572306./-00

-.22994974./-00  +.88923996./-00  -.31233224./-01  +.22880801./-01
+.50224745./-00  +.22994974./-00  +.22880801./-01  +.46953838./-01
+.11541081./-00  +.43745228./-00  +.43559800./-01  -.56976154./-01
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+.10335344./+01  +.27944053./-00  +.50802979./-01  -.11505029./-00
                 +.16788381./+01  -.14818952./-00  -.50802979./-01
                                  +.10000853./+01  -.54648578./-04
                                                   +.99991464./-00
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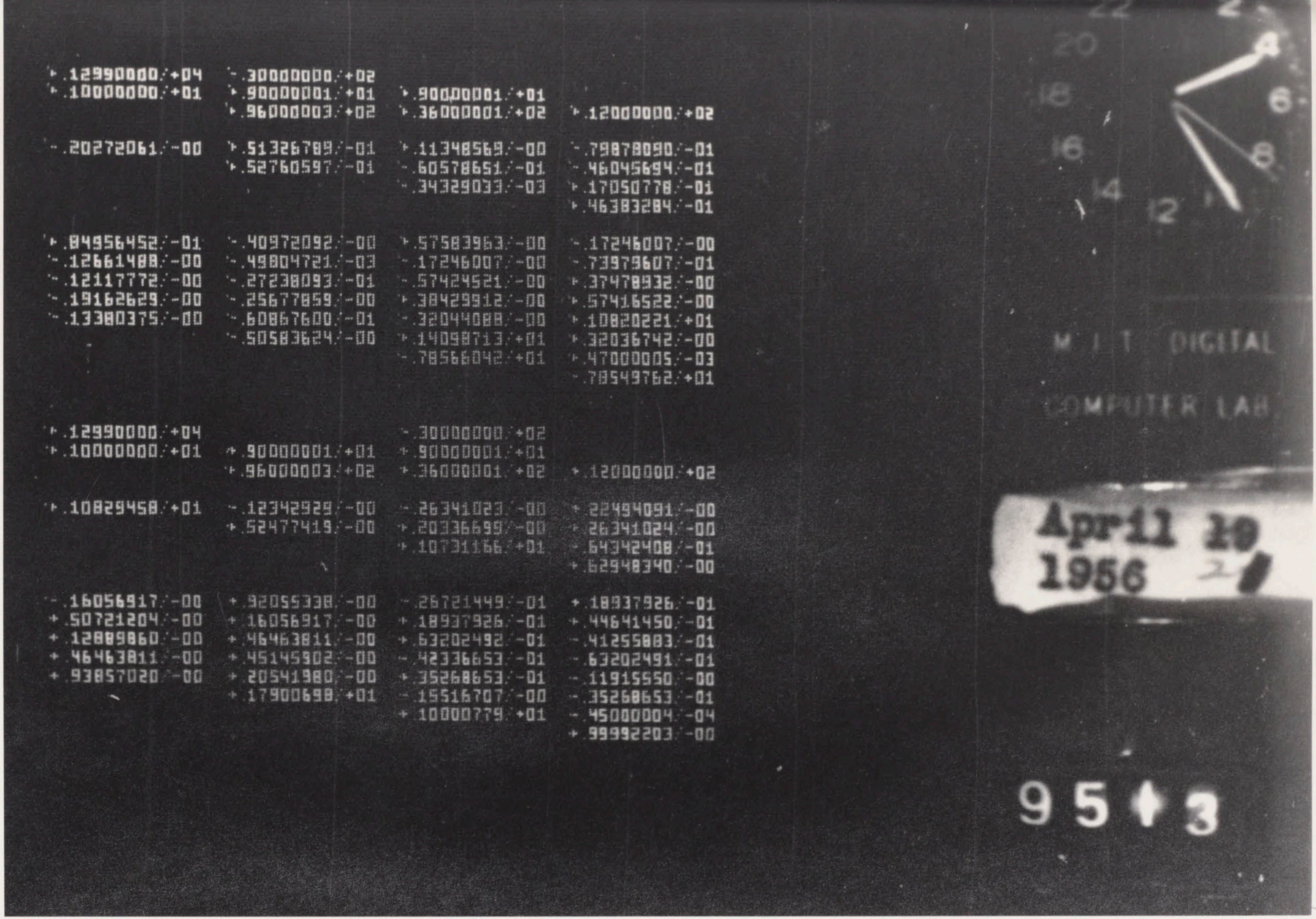
M. I. T. DIGITAL
COMPUTER LA

April 19
1956 2

9507



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+.12990000./+04    -.30000000./+02
+.10000000./+01    +.90000001./+01    +.90000001./+01
                   +.96000003./+02    +.36000001./+02    +.12000000./+02

-.20272061./-00    +.51326789./-01    +.11348569./-00    -.79878090./-01
                   +.52760597./-01    -.60578651./-01    -.46045694./-01
                                      -.34329033./-03    +.17050778./-01
                                                         +.46383284./-01

+.84956452./-01    -.40972092./-00    +.57583963./-00    -.17246007./-00
-.12661488./-00    -.49804721./-03    -.17246007./-00    -.73979607./-01
-.12117772./-00    -.27238093./-01    -.57424521./-00    +.37478932./-00
-.19162629./-00    -.25677859./-00    +.38429912./-00    +.57416522./-00
-.13380375./-00    -.60867600./-01    -.32044088./-00    +.10820221./+01
                   -.50583624./-00    +.14098713./+01    +.32036742./-00
                                      -.78566042./+01    +.47000005./-03
                                                         -.78549762./+01


+.12990000./+04                       -.30000000./+02
+.10000000./+01    +.90000001./+01    +.90000001./+01
                   +.96000003./+02    +.36000001./+02    +.12000000./+02

+.10829458./+01    -.12342929./-00    -.26341023./-00    +.22494091./-00
                   +.52477419./-00    +.20336699./-00    +.26341024./-00
                                      +.10731166./+01    -.64342408./-01
                                                         +.62948340./-00

-.16056917./-00    +.92055338./-00    -.26721449./-01    +.18937926./-01
+.50721204./-00    +.16056917./-00    +.18937926./-01    +.44641450./-01
+.12889860./-00    +.46463811./-00    +.63202492./-01    -.41255883./-01
+.46463811./-00    +.45145902./-00    -.42336653./-01    -.63202491./-01
+.93857020./-00    +.20541980./-00    +.35268653./-01    -.11915550./-00
                   +.17900698./+01    -.15516707./-00    -.35268653./-01
                                      +.10000779./+01    -.45000004./-04
                                                         +.99992203./-00
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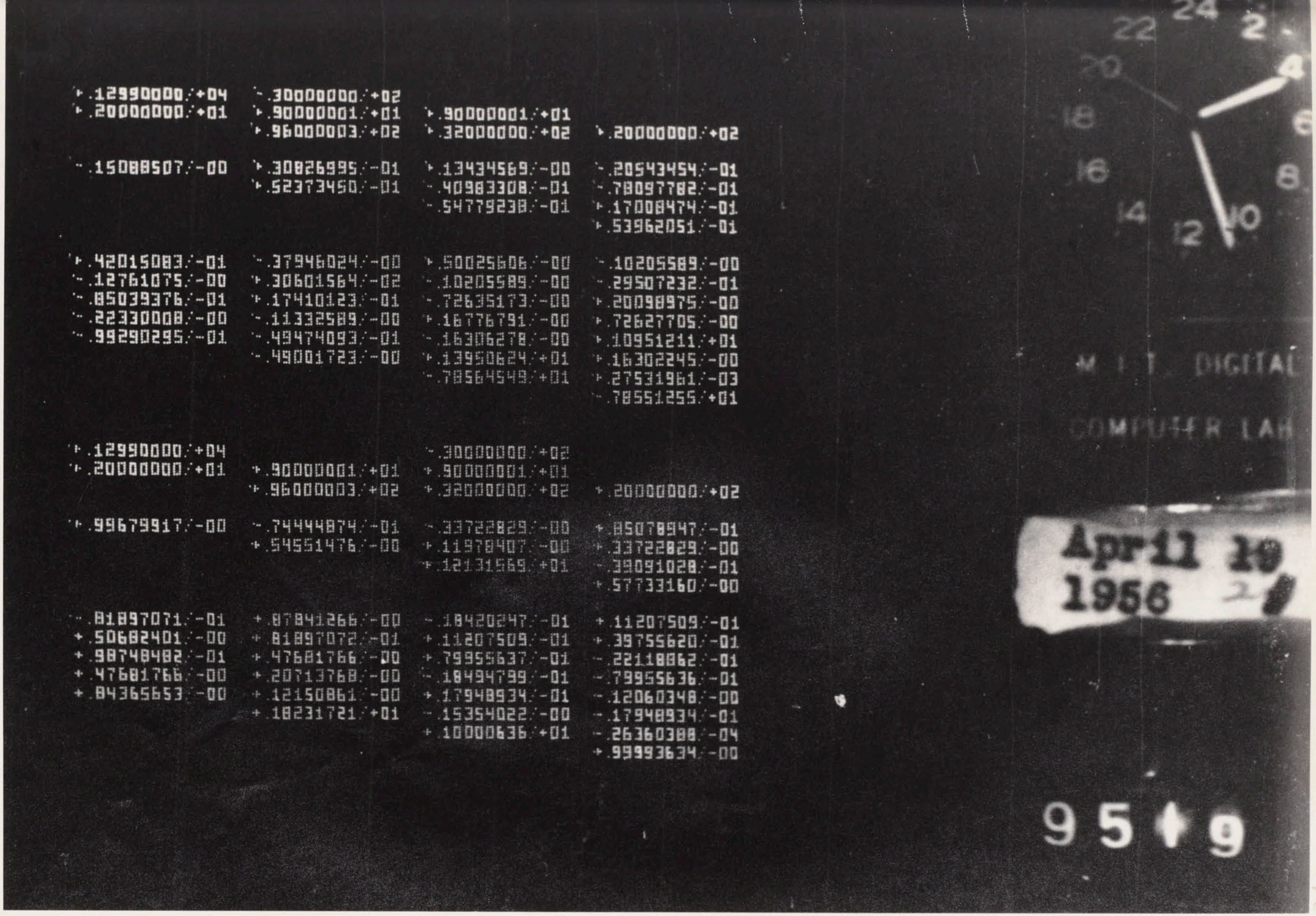

```
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                 +.96000003/+02   +.32000000/+02   +.20000000/+02

-.15088507/-00   +.30826995/-01   +.13434569/-00   -.20543454/-01
                 +.52373450/-01   -.40983308/-01   -.78097782/-01
                                  -.54779238/-01   +.17008474/-01
                                                   +.53962051/-01

+.42015083/-01   -.37946024/-00   +.50025606/-00   -.10205589/-00
-.12761075/-00   +.30601564/-02   -.10205589/-00   -.29507232/-01
-.85039376/-01   +.17410123/-01   -.72635173/-00   +.20098975/-00
-.22330008/-00   -.11332589/-00   +.16776791/-00   +.72627705/-00
-.99290295/-01   -.49474093/-01   -.16306278/-00   +.10951211/+01
                 -.49001723/-00   +.13950624/+01   +.16302245/-00
                                  -.78564549/+01   +.27531961/-03
                                                   -.78551255/+01


+.12990000/+04                    -.30000000/+02
+.20000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.32000000/+02   +.20000000/+02

+.99679917/-00   -.74444874/-01   -.33722829/-00   +.85078947/-01
                 +.54551476/-00   +.11978407/-00   +.33722829/-00
                                  +.12131569/+01   -.39091028/-01
                                                   +.57733160/-00

-.81897071/-01   +.87841266/-00   -.18420247/-01   +.11207509/-01
+.50682401/-00   +.81897072/-01   +.11207509/-01   +.39755620/-01
+.98748482/-01   +.47681766/-00   +.79955637/-01   -.22118862/-01
+.47681766/-00   +.20713768/-00   -.18494799/-01   -.79955636/-01
+.84365653/-00   +.12150861/-00   +.17948934/-01   -.12060348/-00
                 +.18231721/+01   -.15354022/-00   -.17948934/-01
                                  +.10000636/+01   -.26360388/-04
                                                   +.99993634/-00
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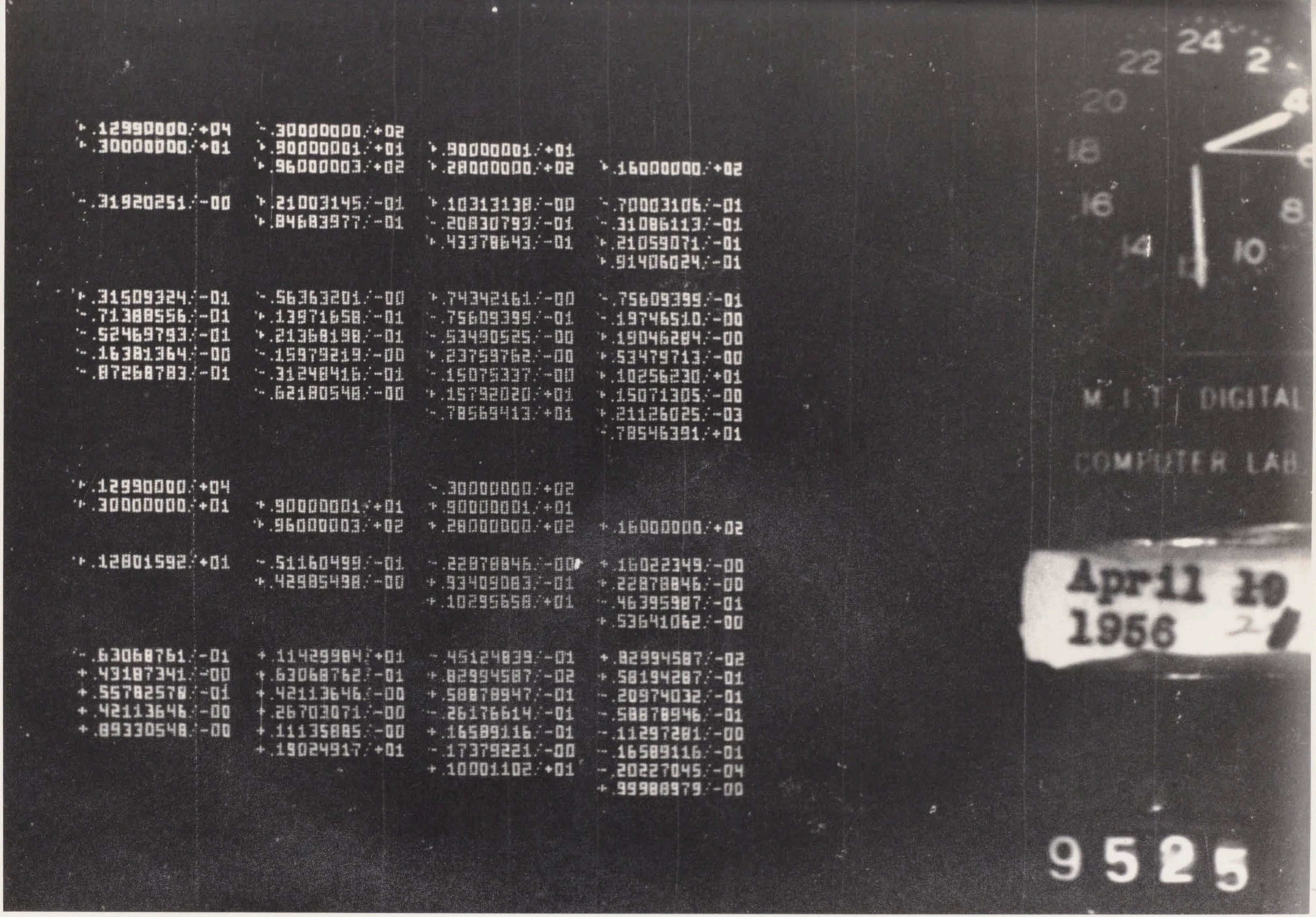
40



```
+.12990000/+04  -.30000000/+02
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                +.96000003/+02  +.28000000/+02  +.16000000/+02

-.31920251/-00  +.21003145/-01  +.10313138/-00  -.70003106/-01
                +.84683977/-01  -.20830793/-01  -.31086113/-01
                                +.43378643/-01  +.21059071/-01
                                                +.91406024/-01

+.31509324/-01  -.56363201/-00  +.74342161/-00  -.75609399/-01
-.71388556/-01  +.13971658/-01  -.75609399/-01  -.19746510/-00
-.52469793/-01  +.21368198/-01  -.53490525/-00  +.19046284/-00
-.16381364/-00  -.15979219/-00  +.23759762/-00  +.53479713/-00
-.87268783/-01  -.31248416/-01  -.15075337/-00  +.10256230/+01
                -.62180548/-00  +.15792020/+01  +.15071305/-00
                                -.78569413/+01  +.21126025/-03
                                                -.78546391/+01


+.12990000/+04                  -.30000000/+02
+.30000000/+01  +.90000001/+01  +.90000001/+01
                +.96000003/+02  +.28000000/+02  +.16000000/+02

+.12801592/+01  -.51160499/-01  -.22878846/-00  +.16022349/-00
                +.42985498/-00  +.93409083/-01  +.22878846/-00
                                +.10295658/+01  -.46395987/-01
                                                +.53641062/-00

-.63068761/-01  +.11429984/+01  -.45124839/-01  +.82994587/-02
+.43187341/-00  +.63068762/-01  +.82994587/-02  +.58194287/-01
+.55782578/-01  +.42113646/-00  +.58878947/-01  -.20974032/-01
+.42113646/-00  +.26703071/-00  -.26176614/-01  -.58878946/-01
+.89330548/-00  +.11135885/-00  +.16589116/-01  -.11297281/-00
                +.19024917/+01  -.17379221/-00  -.16589116/-01
                                +.10001102/+01  -.20227045/-04
                                                +.99988979/-00
```
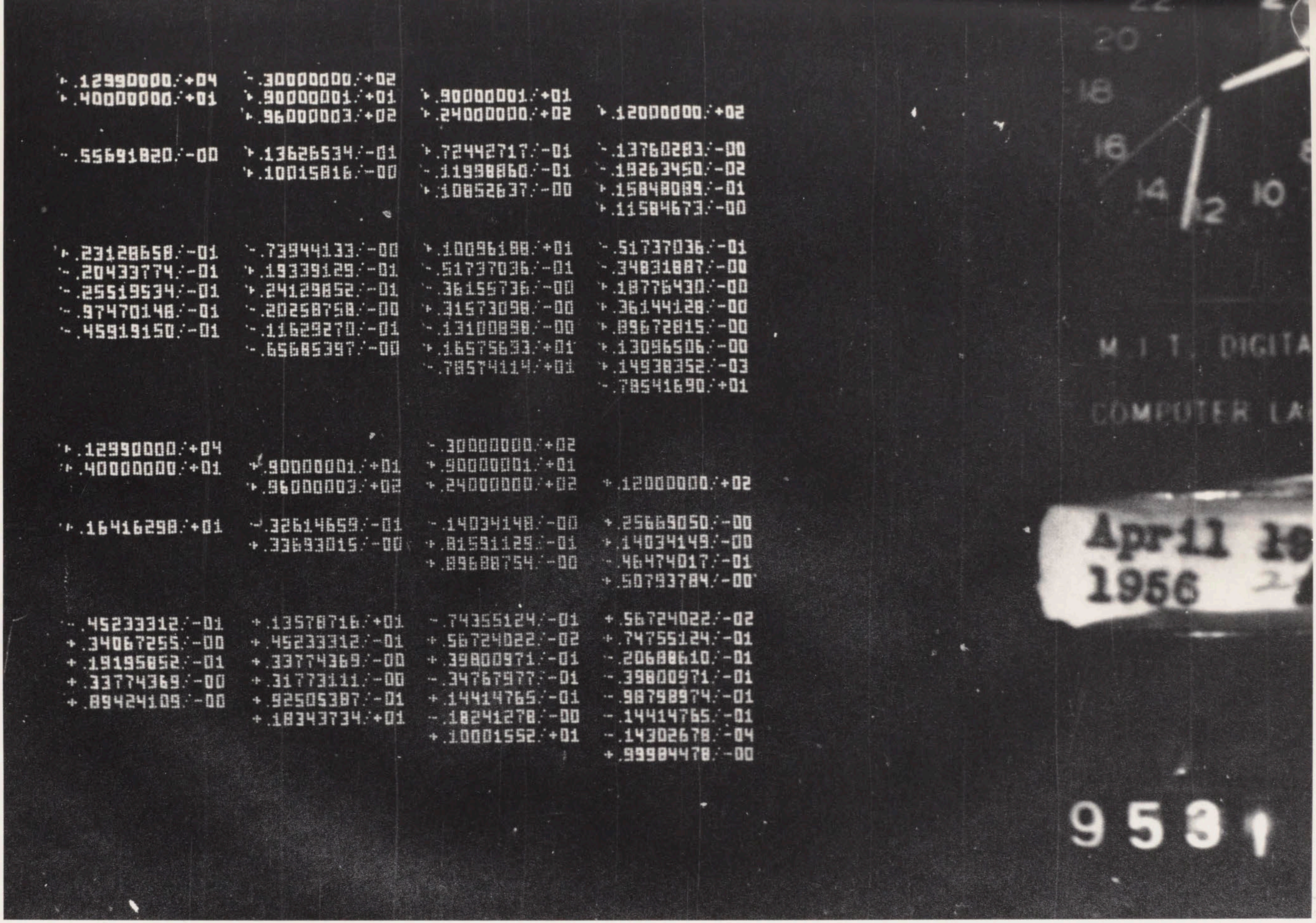

M.I.T. DIGITAL
COMPUTER LAB

April 10
1956

9525



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+.12990000.:+04   -.30000000.:+02
+.40000000.:+01   +.90000001.:+01   +.90000001.:+01
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-.55691820.:-00   +.13626534.:-01   +.72442717.:-01   -.13760283.:-00
                  +.10015816.:-00   -.11998860.:-01   -.19263450.:-02
                                    +.10852637.:-00   +.15848089.:-01
                                                      +.11584673.:-00

+.23128658.:-01   -.73944133.:-00   +.10096188.:+01   -.51737036.:-01
-.20433774.:-01   +.19339129.:-01   -.51737036.:-01   -.34831887.:-00
-.25519534.:-01   +.24129852.:-01   -.36155736.:-00   +.18776430.:-00
-.97470148.:-01   -.20258758.:-00   +.31573098.:-00   +.36144128.:-00
-.45919150.:-01   -.11629270.:-01   -.13100898.:-00   +.89672815.:-00
                  -.65685397.:-00   +.16575633.:+01   +.13096506.:-00
                                    -.78574114.:+01   +.14938352.:-03
                                                      -.78541690.:+01


+.12990000.:+04                     -.30000000.:+02
+.40000000.:+01   +.90000001.:+01   +.90000001.:+01
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+.16416298.:+01   -.32614659.:-01   -.14034148.:-00   +.25669050.:-00
                  +.33693015.:-00   +.81591129.:-01   +.14034149.:-00
                                    +.89680754.:-00   -.46474017.:-01
                                                      +.50793784.:-00

-.45233312.:-01   +.13578716.:+01   -.74355124.:-01   +.56724022.:-02
+.34067255.:-00   +.45233312.:-01   +.56724022.:-02   +.74755124.:-01
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+.89424109.:-00   +.92505387.:-01   +.14414765.:-01   -.98798974.:-01
                  +.18343734.:+01   -.18241278.:-00   -.14414765.:-01
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                                                      +.99984478.:-00
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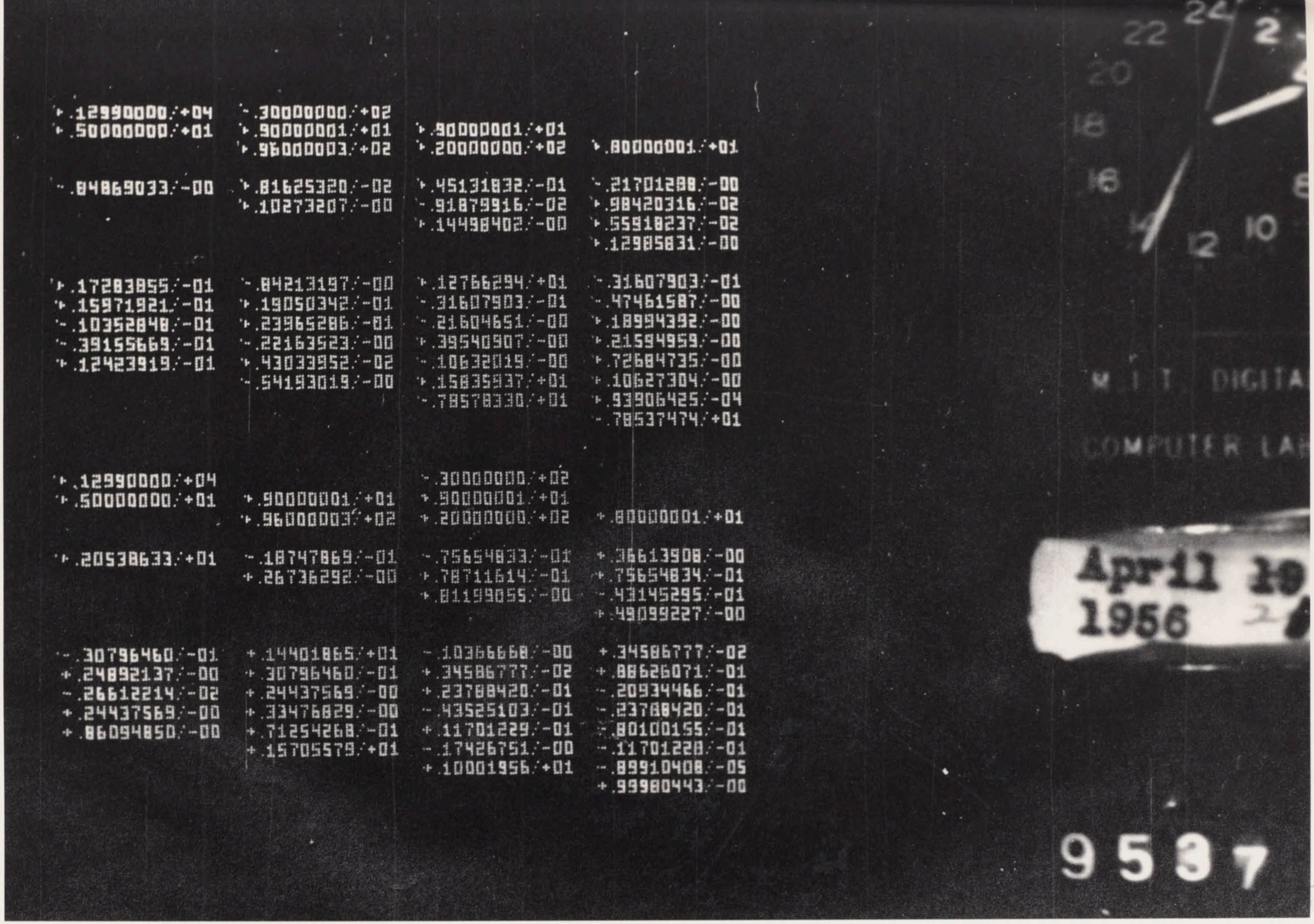

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+.12990000./+04   -.30000000./+02
+.50000000./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.20000000./+02   +.80000001./+01

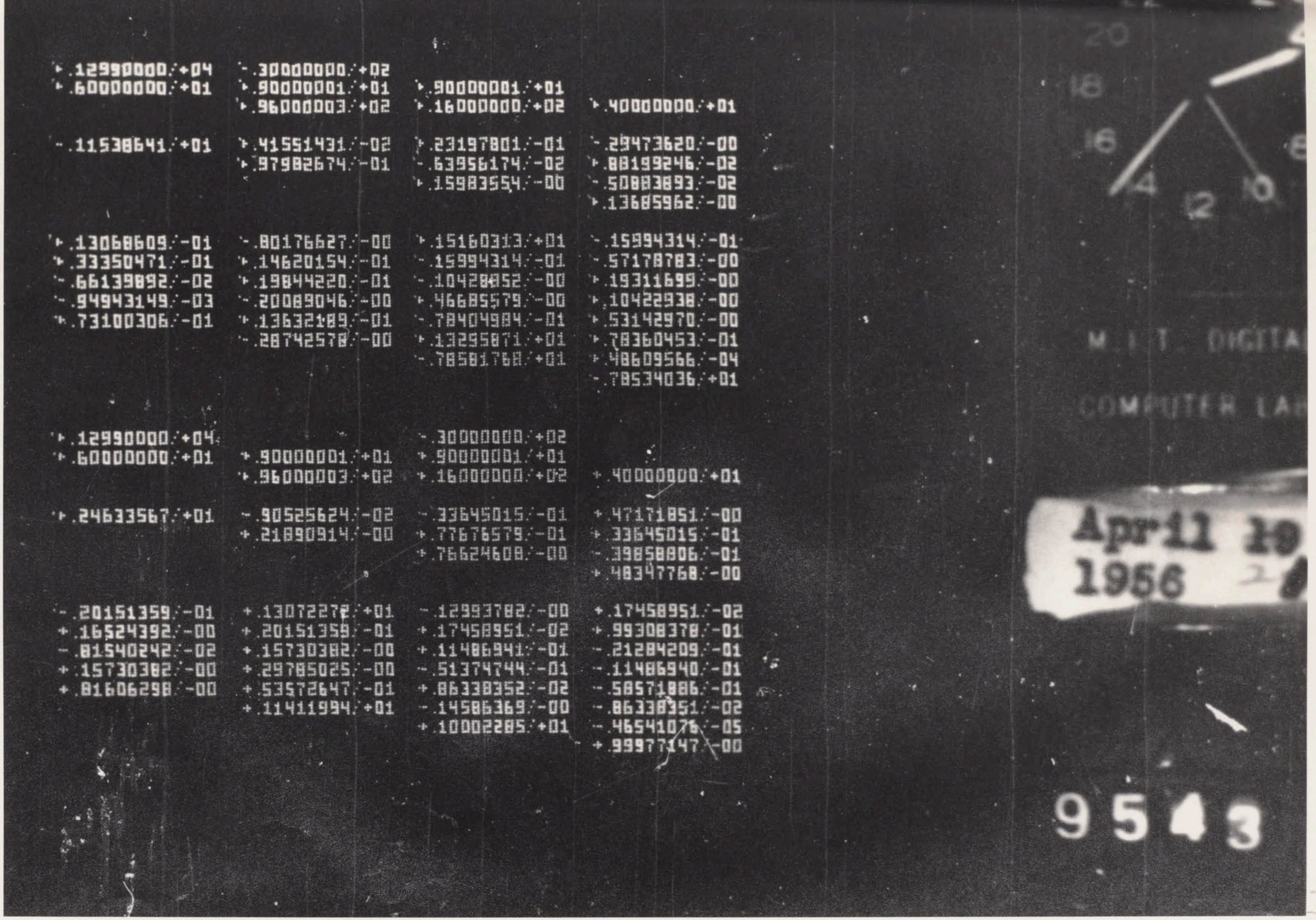
-.84869033./-00   +.81625320./-02   +.45131832./-01   -.21701288./-00
                  +.10273207./-00   -.91879916./-02   +.98420316./-02
                                    +.14498402./-00   +.55918237./-02
                                                      +.12985831./-00

+.17283855./-01   -.84213197./-00   +.12766294./+01   -.31607903./-01
+.15971921./-01   +.19050342./-01   -.31607903./-01   -.47461587./-00
-.10352848./-01   +.23965286./-01   -.21604651./-00   +.18994392./-00
-.39155669./-01   -.22163523./-00   +.39540907./-00   +.21594959./-00
+.12423919./-01   +.43033952./-02   -.10632019./-00   +.72684735./-00
                  -.54193019./-00   +.15835937./+01   +.10627304./-00
                                    -.78578330./+01   +.93906425./-04
                                                      -.78537474./+01


+.12990000./+04                     -.30000000./+02
+.50000000./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.20000000./+02   +.80000001./+01

+.20538633./+01   -.18747869./-01   -.75654833./-01   +.36613908./-00
                  +.26736292./-00   +.78711614./-01   +.75654834./-01
                                    +.81199055./-00   -.43145295./-01
                                                      +.49099227./-00

-.30796460./-01   +.14401865./+01   -.10366668./-00   +.34586777./-02
+.24892137./-00   +.30796460./-01   +.34586777./-02   +.88626071./-01
-.26612214./-02   +.24437569./-00   +.23788420./-01   -.20934466./-01
+.24437569./-00   +.33476829./-00   -.43525103./-01   -.23788420./-01
+.86094850./-00   +.71254268./-01   +.11701229./-01   -.80100155./-01
                  +.15705579./+01   -.17426751./-00   -.11701228./-01
                                    +.10001956./+01   -.89910408./-05
                                                      +.99980443./-00
```



```
+.12990000./+04   -.30000000./+02
+.60000000./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.16000000./+02   +.40000000./+01

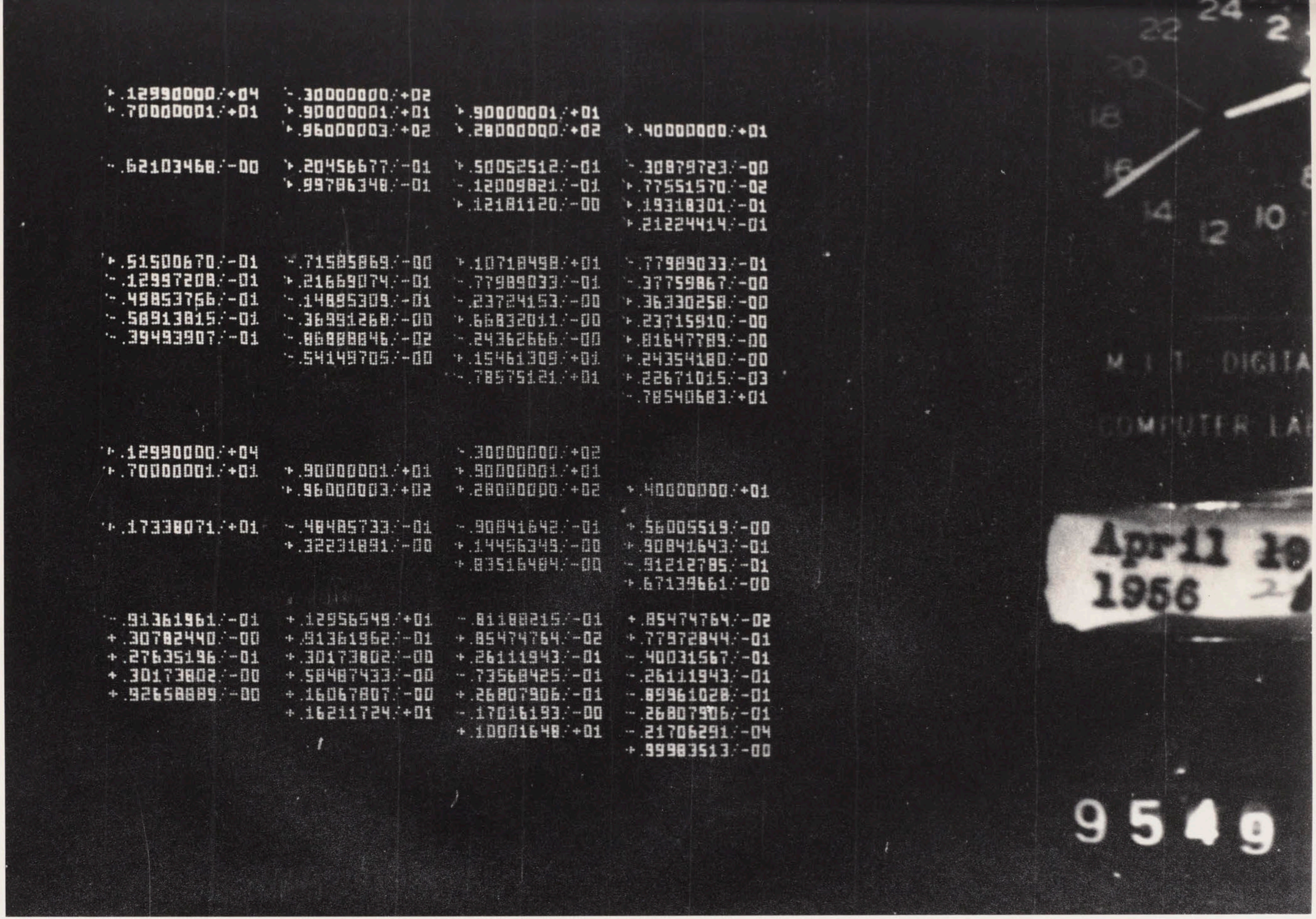
-.11538641./+01   +.41551431./-02   +.23197801./-01   -.29473620./-00
                  +.97982674./-01   -.63956174./-02   +.88199246./-02
                                    +.15983554./-00   -.50883893./-02
                                                      +.13685962./-00

+.13068609./-01   -.80176627./-00   +.15160313./+01   -.15994314./-01
+.33350471./-01   +.14620154./-01   -.15994314./-01   -.57178783./-00
-.66139892./-02   +.19844220./-01   -.10428852./-00   +.19311699./-00
-.94943149./-03   -.20089046./-00   +.46685579./-00   +.10422938./-00
+.73100306./-01   +.13632189./-01   -.78404984./-01   +.53142970./-00
                  -.28742578./-00   +.13295871./+01   +.78360453./-01
                                    -.78581768./+01   +.48609566./-04
                                                      -.78534036./+01


+.12990000./+04                     -.30000000./+02
+.60000000./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.16000000./+02   +.40000000./+01

+.24633567./+01   -.90525624./-02   -.33645015./-01   +.47171851./-00
                  +.21890914./-00   +.77676579./-01   +.33645015./-01
                                    +.76624608./-00   -.39858806./-01
                                                      +.48347768./-00

-.20151359./-01   +.13072272./+01   -.12993782./-00   +.17458951./-02
+.16524392./-00   +.20151359./-01   +.17458951./-02   +.99308378./-01
-.81540242./-02   +.15730382./-00   +.11486941./-01   -.21284209./-01
+.15730382./-00   +.29785025./-00   -.51374744./-01   -.11486940./-01
+.81606298./-00   +.53572647./-01   +.86338352./-02   -.58571886./-01
                  +.11411994./+01   -.14586369./-00   -.86338351./-02
                                    +.10002285./+01   -.46541076./-05
                                                      +.99977147./-00
```



```
+.12990000/+04    -.30000000/+02
+.70000001/+01    +.90000001/+01    +.90000001/+01
                  +.96000003/+02    +.28000000/+02    +.40000000/+01

-.62103468/-00    +.20456677/-01    +.50052512/-01    -.30879723/-00
                  +.99786348/-01    -.12009821/-01    +.77551570/-02
                                    +.12181120/-00    +.19318301/-01
                                                      +.21224414/-01

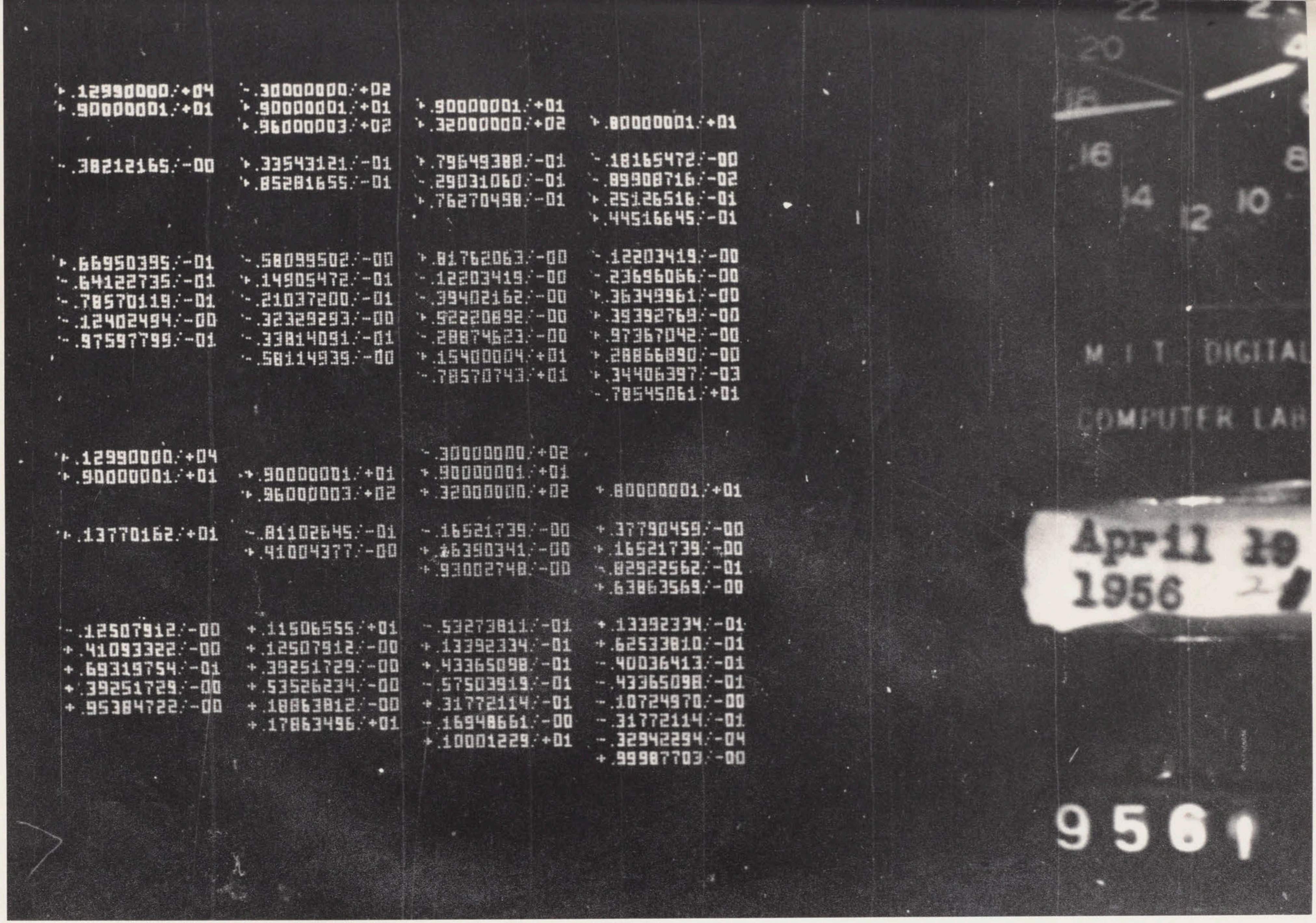
+.51500670/-01    -.71585869/-00    +.10718498/+01    -.77989033/-01
-.12997208/-01    +.21669074/-01    -.77989033/-01    -.37759867/-00
-.49853766/-01    -.14895309/-01    -.23724153/-00    +.36330258/-00
-.58913815/-01    -.36991268/-00    +.66832011/-00    +.23715910/-00
-.39493907/-01    -.86888846/-02    -.24362666/-00    +.81647789/-00
                  -.54149705/-00    +.15461309/+01    +.24354180/-00
                                    -.78575121/+01    +.22671015/-03
                                                      -.78540683/+01


+.12990000/+04                      -.30000000/+02
+.70000001/+01    +.90000001/+01    +.90000001/+01
                  +.96000003/+02    +.28000000/+02    +.40000000/+01

+.17338071/+01    -.48485733/-01    -.90841642/-01    +.56005519/-00
                  +.32231891/-00    +.14456349/-00    +.90841643/-01
                                    +.83516484/-00    -.91212785/-01
                                                      +.67139661/-00

-.91361961/-01    +.12956549/+01    -.81188215/-01    +.85474764/-02
+.30782440/-00    +.91361962/-01    +.85474764/-02    +.77972844/-01
+.27635196/-01    +.30173802/-00    +.26111943/-01    -.40031567/-01
+.30173802/-00    +.58487433/-00    -.73568425/-01    -.26111943/-01
+.92658889/-00    +.16067807/-00    +.26807906/-01    -.89961028/-01
                  +.16211724/+01    -.17016193/-00    -.26807906/-01
                                    +.10001648/+01    -.21706291/-04
                                                      +.99983513/-00
```

45



```
+.12990000./+04   -.30000000./+02
+.90000001./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.32000000./+02   +.80000001./+01

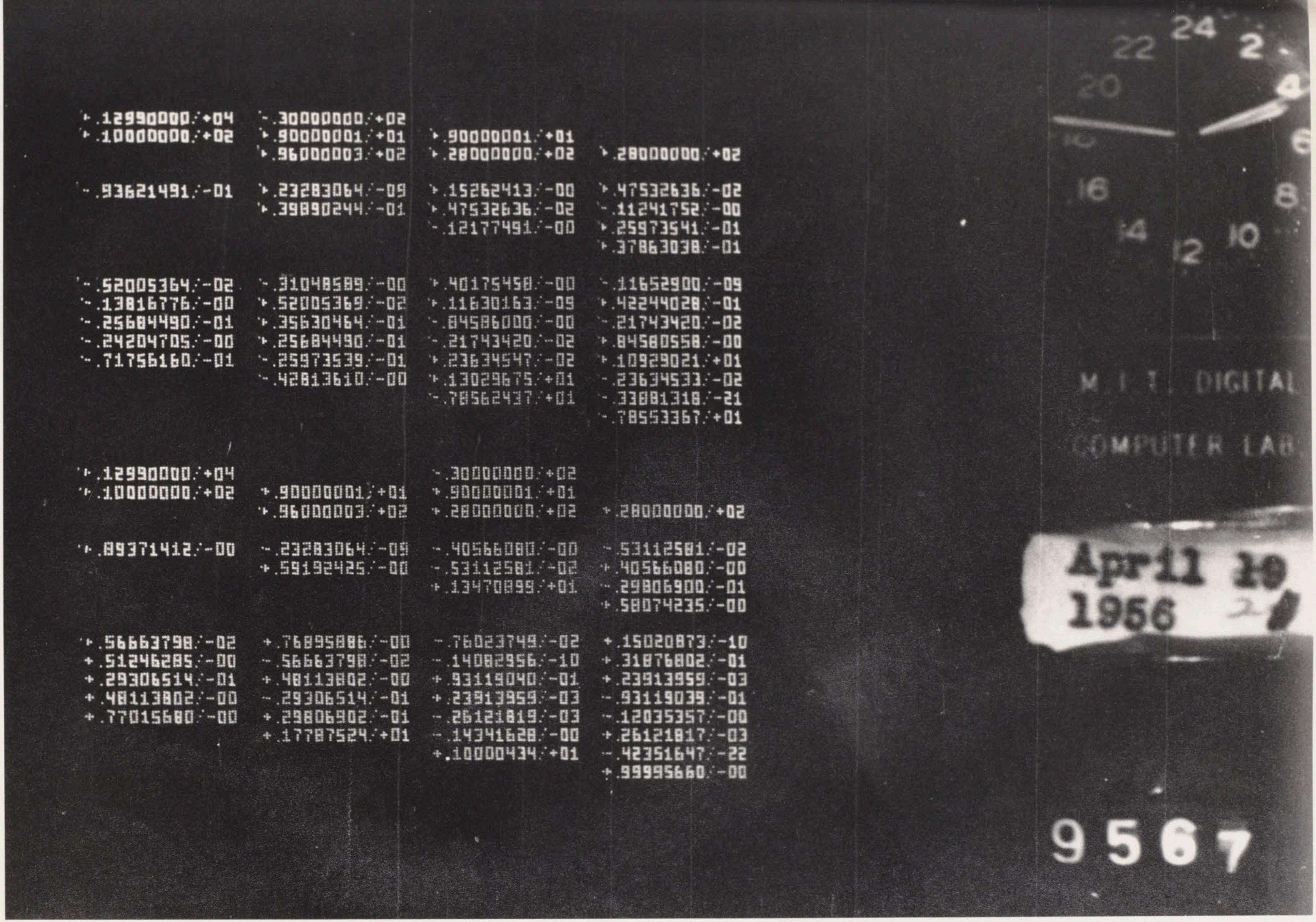
-.38212165./-00   +.33543121./-01   +.79649388./-01   -.18165472./-00
                  +.85281655./-01   -.29031060./-01   -.89908716./-02
                                    +.76270498./-01   +.25126516./-01
                                                      +.44516645./-01

+.66950395./-01   -.58099502./-00   +.81762063./-00   -.12203419./-00
-.64122735./-01   +.14905472./-01   -.12203419./-00   -.23696066./-00
-.78570119./-01   -.21037200./-01   -.39402162./-00   +.36349961./-00
-.12402494./-00   -.32329293./-00   +.92220892./-00   +.39392769./-00
-.97597799./-01   -.33814091./-01   -.28874623./-00   +.97367042./-00
                  -.58114939./-00   +.15400004./+01   +.28866890./-00
                                    -.78570743./+01   +.34406397./-03
                                                      -.78545061./+01

+.12990000./+04                     -.30000000./+02
+.90000001./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.32000000./+02   +.80000001./+01

+.13770162./+01   -.81102645./-01   -.16521739./-00   +.37790459./-00
                  +.41004377./-00   +.86390341./-00   +.16521739./-00
                                    +.93002748./-00   -.82922562./-01
                                                      +.63863569./-00

-.12507912./-00   +.11506555./+01   -.53273811./-01   +.13392334./-01
+.41093322./-00   +.12507912./-00   +.13392334./-01   +.62533810./-01
+.69319754./-01   +.39251729./-00   +.43365098./-01   -.40036413./-01
+.39251729./-00   +.53526234./-00   -.57503919./-01   -.43365098./-01
+.95384722./-00   +.18863812./-00   +.31772114./-01   -.10724970./-00
                  +.17863496./+01   -.16948661./-00   -.31772114./-01
                                    +.10001229./+01   -.32942294./-04
                                                      +.99987703./-00
```



```
+.12990000/+04   -.30000000/+02
+.10000000/+02   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.28000000/+02   +.28000000/+02

-.93621491/-01   +.23283064/-09   +.15262413/-00   +.47532636/-02
                 +.39890244/-01   +.47532636/-02   -.11241752/-00
                                  -.12177491/-00   +.25973541/-01
                                                   +.37863038/-01

-.52005364/-02   -.31048589/-00   +.40175458/-00   -.11652900/-09
-.13816776/-00   +.52005369/-02   +.11630163/-09   +.42244028/-01
-.25684490/-01   +.35630464/-01   -.84586000/-00   -.21743420/-02
-.24204705/-00   +.25684490/-01   -.21743420/-02   +.84580558/-00
-.71756160/-01   -.25973539/-01   +.23634547/-02   +.10929021/+01
                 -.42813610/-00   +.13029675/+01   -.23634533/-02
                                  -.78562437/+01   -.33081318/-21
                                                   -.78553367/+01


+.12990000/+04                    -.30000000/+02
+.10000000/+02   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.28000000/+02   +.28000000/+02

+.89371412/-00   -.23283064/-09   -.40566080/-00   -.53112581/-02
                 +.59192425/-00   -.53112581/-02   +.40566080/-00
                                  +.13470899/+01   -.29806900/-01
                                                   +.58074235/-00

+.56663798/-02   +.76895886/-00   -.76023749/-02   +.15020873/-10
+.51246285/-00   -.56663798/-02   -.14082956/-10   +.31876802/-01
+.29306514/-01   +.48113802/-00   +.93119040/-01   +.23913959/-03
+.48113802/-00   -.29306514/-01   +.23913959/-03   -.93119039/-01
+.77015680/-00   +.29806902/-01   -.26121819/-03   -.12035357/-00
                 +.17787524/+01   -.14341628/-00   +.26121817/-03
                                  +.10000434/+01   -.42351647/-22
                                                   +.99995660/-00
```

M.I.T. DIGITAL

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April 19
1956 2

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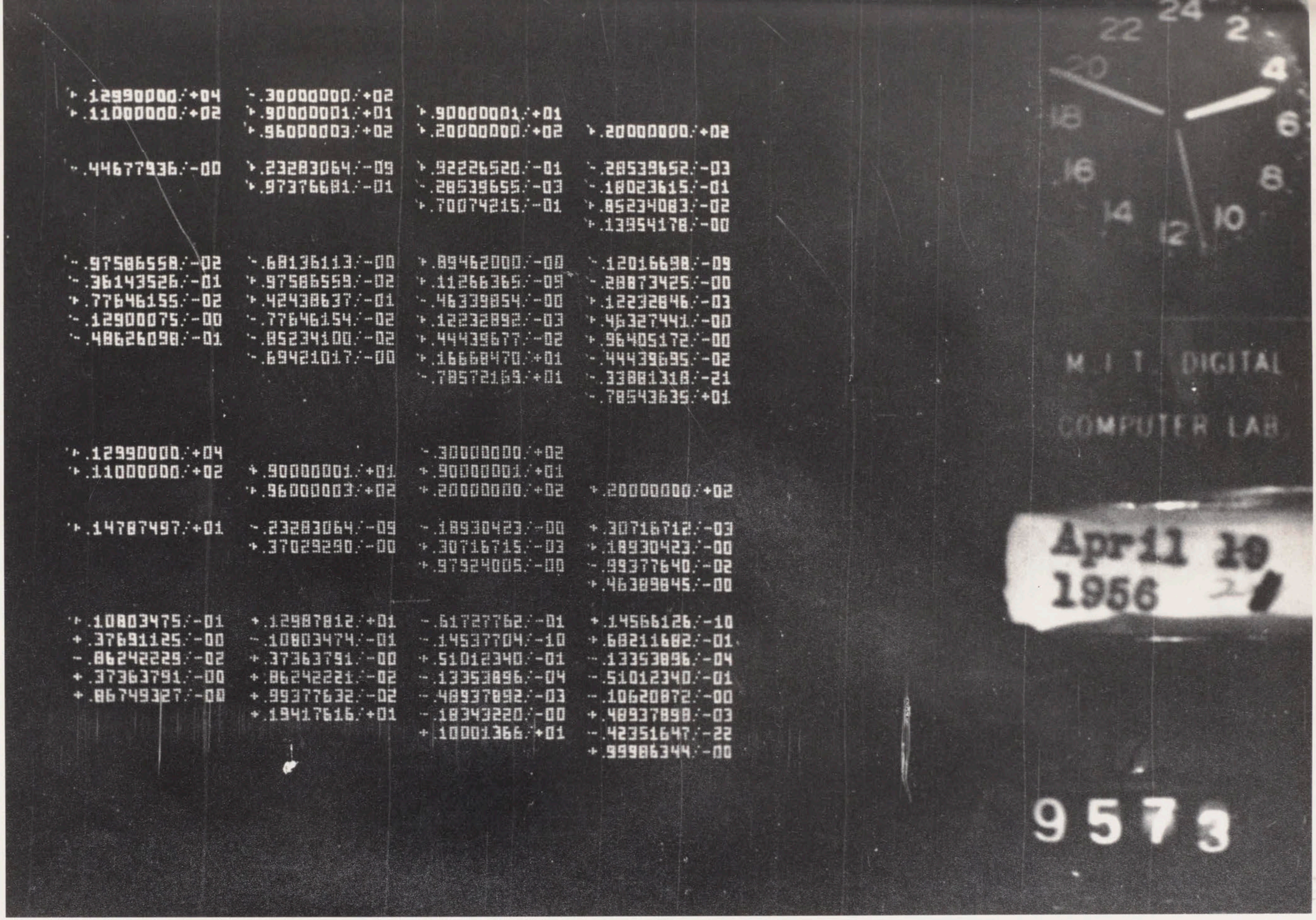


```
+.12990000./+04   -.30000000./+02
+.11000000./+02   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.20000000./+02   +.20000000./+02

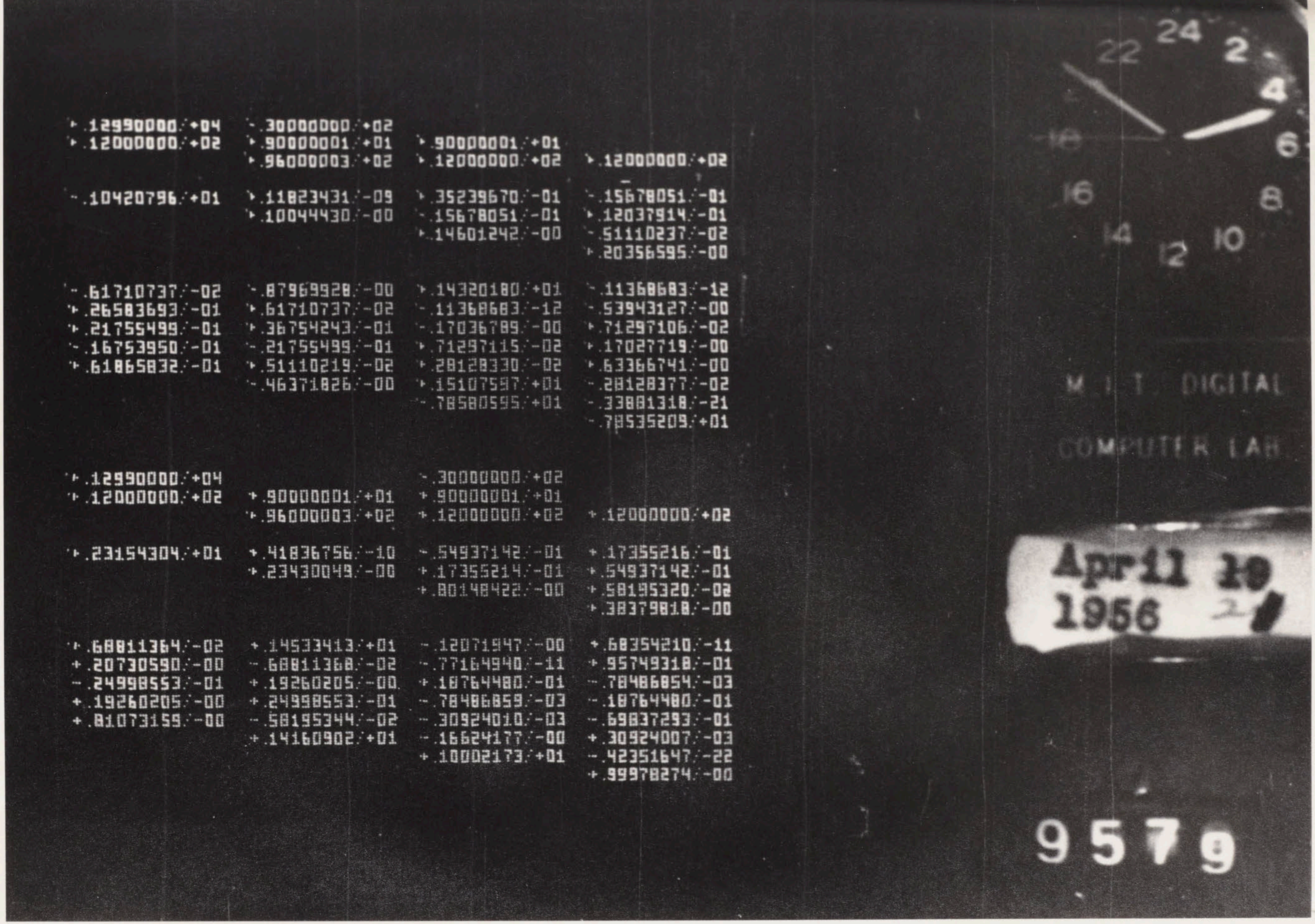
-.44677936./-00   +.23283064./-09   +.92226520./-01   -.28539652./-03
                  +.97376681./-01   -.28539655./-03   -.18023615./-01
                                    +.70074215./-01   +.85234083./-02
                                                      +.13954178./-00

-.97586558./-02   -.68136113./-00   +.89462000./-00   -.12016698./-09
-.36143526./-01   +.97586559./-02   +.11266365./-09   -.28873425./-00
+.77646155./-02   +.42438637./-01   -.46339854./-00   +.12232846./-03
-.12900075./-00   -.77646154./-02   +.12232892./-03   +.46327441./-00
-.48626098./-01   -.85234100./-02   +.44439677./-02   +.96405172./-00
                  -.69421017./-00   +.16668470./+01   -.44439695./-02
                                    -.78572169./+01   -.33881318./-21
                                                      -.78543635./+01


+.12990000./+04                     -.30000000./+02
+.11000000./+02   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.20000000./+02   +.20000000./+02

+.14787497./+01   -.23283064./-09   -.18930423./-00   +.30716712./-03
                  +.37029290./-00   +.30716715./-03   +.18930423./-00
                                    +.97924005./-00   -.99377640./-02
                                                      +.46389845./-00

+.10803475./-01   +.12987812./+01   -.61727762./-01   +.14566126./-10
+.37691125./-00   -.10803474./-01   -.14537704./-10   +.68211682./-01
-.86242229./-02   +.37363791./-00   +.51012340./-01   -.13353896./-04
+.37363791./-00   +.86242221./-02   -.13353896./-04   -.51012340./-01
+.86749327./-00   +.99377632./-02   -.48937892./-03   -.10620872./-00
                  +.19417616./+01   -.18343220./-00   +.48937898./-03
                                    +.10001366./+01   -.42351647./-22
                                                      +.99986344./-00
```



```
+.12990000/+04   -.30000000/+02
+.12000000/+02   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.12000000/+02   +.12000000/+02

-.10420796/+01   +.11823431/-09   +.35239670/-01   -.15678051/-01
                 +.10044430/-00   -.15678051/-01   +.12037914/-01
                                  +.14601242/-00   -.51110237/-02
                                                   +.20356595/-00

-.61710737/-02   -.87969928/-00   +.14320180/+01   -.11368683/-12
+.26583693/-01   +.61710737/-02   -.11368683/-12   -.53943127/-00
+.21755499/-01   +.36754243/-01   -.17036789/-00   +.71297106/-02
-.16753950/-01   -.21755499/-01   +.71297115/-02   +.17027719/-00
+.61865832/-01   +.51110219/-02   +.28128330/-02   +.63366741/-00
                 -.46371826/-00   +.15107597/+01   -.28128377/-02
                                  -.78580595/+01   -.33881318/-21
                                                   -.78535209/+01


+.12990000/+04                    -.30000000/+02
+.12000000/+02   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.12000000/+02   +.12000000/+02

+.23154304/+01   +.41836756/-10   -.54937142/-01   +.17355216/-01
                 +.23430049/-00   +.17355214/-01   +.54937142/-01
                                  +.80148422/-00   +.58195320/-02
                                                   +.38379818/-00

+.68811364/-02   +.14533413/+01   -.12071947/-00   +.68354210/-11
+.20730590/-00   -.68811368/-02   -.77164940/-11   +.95749318/-01
-.24998553/-01   +.19260205/-00   +.18764480/-01   -.78486854/-03
+.19260205/-00   +.24998553/-01   -.78486859/-03   -.18764480/-01
+.81073159/-00   -.58195344/-02   -.30924010/-03   -.69837293/-01
                 +.14160902/+01   -.16624177/-00   +.30924007/-03
                                  +.10002173/+01   -.42351647/-22
                                                   +.99978274/-00
```

```
+.12990000./+04  -.30000000./+02
+.13000000./+02  +.90000001./+01  +.90000001./+01
                 +.96000003./+02  +.40000000./+01  +.40000000./+01

-.15608165./+01  +.43655745./-10  +.39078718./-02  -.11041865./-01
                 +.87056301./-01  -.11041865./-01  +.28698658./-02
                                  +.15996155./-00  -.43139285./-02
                                                   +.23245006./-00

-.87452539./-03  -.43307807./-00  +.17958451./+01  -.29217517./-10
+.19102532./-01  +.87452516./-03  +.28990143./-10  -.67040395./-00
+.44084149./-02  +.14921604./-01  -.18906770./-01  +.50040357./-02
+.12512301./-01  -.44084149./-02  +.50040362./-02  +.18892928./-01
+.14858295./-00  +.43139271./-02  +.39880158./-03  +.21837255./-00
                 +.12200497./-00  +.62639057./-00  -.39880943./-03
                                  -.78585463./+01  -.84703294./-22
                                                   -.78530341./+01


+.12990000./+04                   -.30000000./+02
+.13000000./+02  +.90000001./+01  +.90000001./+01
                 +.96000003./+02  +.40000000./+01  +.40000000./+01

+.29875409./+01  -.43655745./-10  -.48787929./-02  +.12271068./-01
                 +.17390768./-00  +.12271068./-01  +.48787933./-02
                                  +.75015836./-00  +.49743209./-02
                                                   +.34993004./-00

+.97873701./-03  +.67428511./-00  -.16062959./-00  +.37374547./-11
+.65503321./-01  -.97873701./-03  -.35385028./-11  +.11016678./-00
-.51378649./-02  +.50722979./-01  +.20840603./-02  -.54978456./-03
+.50722979./-01  +.51378654./-02  -.54978456./-03  -.20840603./-02
+.75262326./-00  -.49743223./-02  -.43807252./-04  -.24066133./-01
                 +.51342743./-00  -.68913727./-01  +.43807253./-04
                                  +.10002638./+01  -.10587911./-22
                                                   +.99973613./-00
```

```
+.10990000 +04   -.30000000 +02   -.30000000 +02   +.30000000 +01
+.56843418 -14   +.90000001 +01   +.90000001 +01
                 +.96000003 +02   +.48000001 +02   +.56843418 -14

+.10424523 +01   +.11817020 -00
                 +.11789034 +01

+.10990000 +04   -.30000000 +02   -.30000000 +02   +.50000000 +01
+.56843418 -14   +.90000001 +01   +.90000001 +01
                 +.96000003 +02   +.48000001 +02   +.56843418 -14

+.22107408 -00   +.88290929 -01
                 +.32902365 -00

+.10990000 +04   -.30000000 +02   -.30000000 +02   +.60000000 +01
+.56843418 -14   +.90000001 +01   +.90000001 +01
                 +.96000003 +02   +.48000001 +02   +.56843418 -14

+.86602538 -00   +.50000000 -00
+.50000000 -00   +.86602538 -00

+.10990000 +04   -.30000000 +02   -.30000000 +02
+.56843418 -14   +.90000001 +01   +.90000001 +01
                 +.96000003 +02   +.48000001 +02   +.56843418 -14

+.17609928 -00                    +.84370505 -00   +.62356454 -00
+.37999844 -00                    -.48711332 -00   +.10800454 +01
```

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23 Mar.
all Data
#1

```
+.10990000/+04   -.30000000/+02   -.30000000/+02   +.30000000/+01
+.10000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.44000001/+02   +.80000001/+01

+.10480194/+01   +.11141113/-00
                 +.11766659/+01

+.10990000/+04   -.30000000/+02   -.30000000/+02   +.50000000/+01
+.10000000/+01   +.90000001/+01   +.90000001/+01
                 +.96800003/+02   +.44000001/+02   +.80000001/+01

+.23111328/-00   +.83424046/-01
                 +.32744306/-00

+.10990000/+04   -.30000000/+02   -.30000000/+02   +.60000000/+01
+.10000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.44000001/+02   +.80000001/+01

+.86602538/-00   +.50000006/-00
-.50000005/-00   +.86602538/-00

+.10990000/+04   -.30000000/+02   -.30000000/+02
+.10000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.44000001/+02   +.80000001/+01

+.18294838/-00                    +.85190582/-00   +.62049466/-00
+.37560796/-00                    -.49189814/-00   +.10747201/+01
```

23 Mar.
all Data
#1

```
+.10990000./+04   +.30000000./+02   -.30000000./+02   +.30000000./+01
+.20000000./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.40000001./+02   +.16000000./+02

+.10640182./+01   +.90363549./-01
                  +.11683615./+01


+.10990000./+04   -.30000000./+02   -.30000000./+02   +.50000000./+01
+.20000000./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.40000001./+02   +.16000000./+02

+.24271412./-00   +.68036019./-01
                  +.32127535./-00


+.10990000./+04   -.30000000./+02   +.30000000./+02   +.60000000./+01
+.20000000./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.40000001./+02   +.16000000./+02

+.86602538./-00   +.50000000./-00
-.50000000./-00   +.86602538./-00

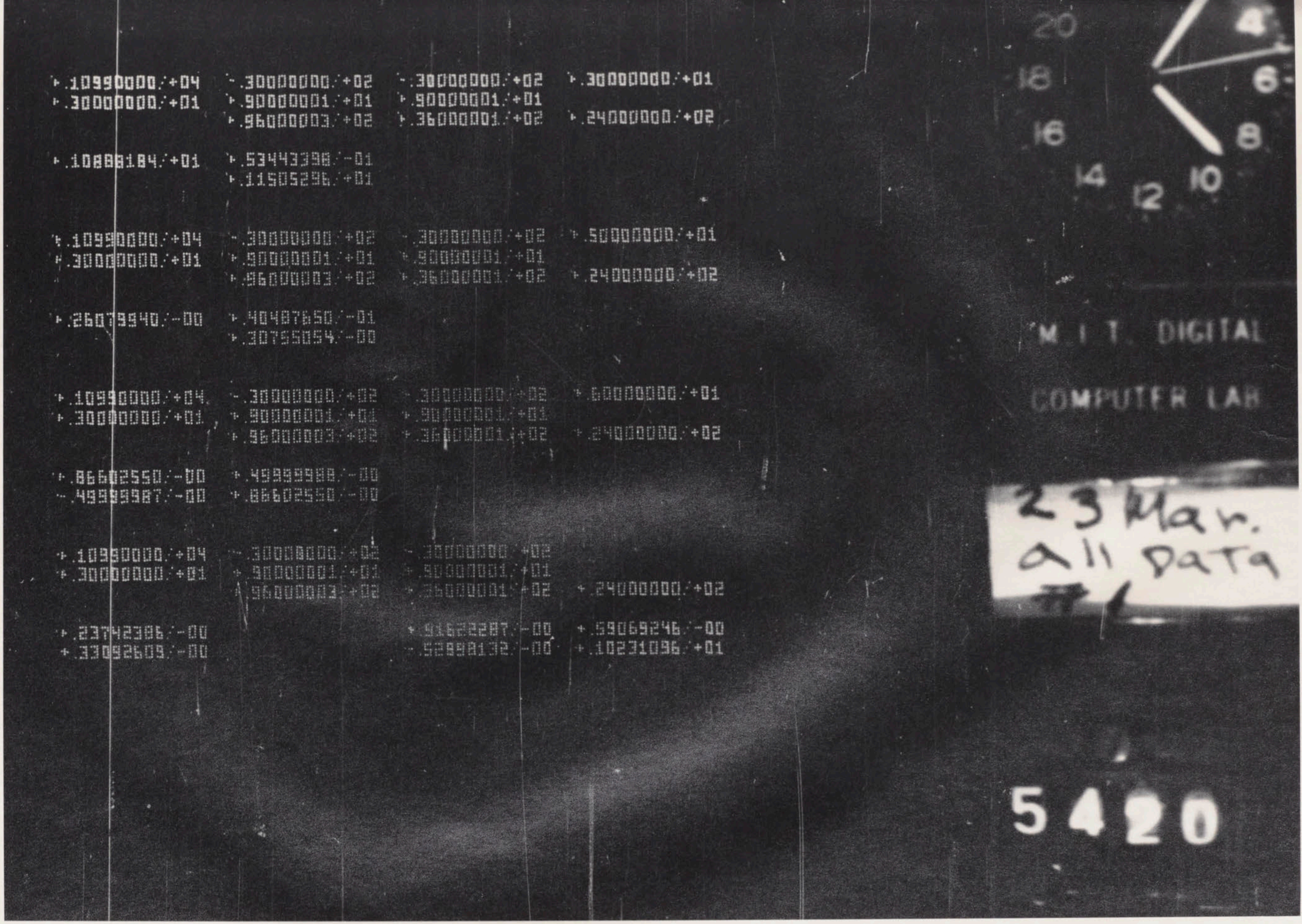

+.10990000./+04   -.30000000./+02   -.30000000./+02
+.20000000./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.40000001./+02   +.16000000./+02

+.20343351./-00                     +.87628483./-00   +.61026662./-00
+.36055597./-00                     -.50592327./-00   +.10570126./+01
```

M.I.T. DIGITAL
COMPUTER LAB

23 Mar.
all Data
#1

5418



```
+.10990000/+04   -.30000000/+02   -.30000000/+02   +.30000000/+01
+.30000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.36000001/+02   +.24000000/+02

+.10888184/+01   +.53443398/-01
                 +.11505296/+01


+.10990000/+04   -.30000000/+02   -.30000000/+02   +.50000000/+01
+.30000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.36000001/+02   +.24000000/+02

+.26079940/-00   +.40487650/-01
                 +.30755054/-00


+.10990000/+04   -.30000000/+02   -.30000000/+02   +.60000000/+01
+.30000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.36000001/+02   +.24000000/+02

+.86602550/-00   +.49999988/-00
-.49999987/-00   +.86602550/-00


+.10990000/+04   -.30000000/+02   -.30000000/+02
+.30000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.36000001/+02   +.24000000/+02

+.23742386/-00                    +.91622287/-00   +.59069246/-00
+.33092609/-00                    -.52898132/-00   +.10231096/+01
```

```
+.10990000./+04  -.30000000./+02  -.30000000./+02  +.30000000./+01
+.40000000./+01  +.90000001./+01  +.90000001./+01
                 +.96000003./+02  +.32000000./+02  +.32000000./+02

+.11209030./+01  +.16155871./-27
                 +.11209030./+01


+.10990000./+04  -.30000000./+02  -.30000000./+02  +.50000000./+01
+.40000000./+01  +.90000001./+01  +.90000001./+01
                 +.96000003./+02  +.32000000./+02  +.32000000./+02

+.28475585./-00  +.69705345./-10
                 +.28475585./-00


+.10990000./+04  -.30000000./+02  -.30000000./+02  +.60000000./+01
+.40000000./+01  +.90000001./+01  +.90000001./+01
                 +.96000003./+02  +.32000000./+02  +.32000000./+02

+.10000000./+01  +.16155871./-27
+.16155871./-27  +.10000000./+01


+.10990000./+04  -.30000000./+02  -.30000000./+02
+.40000000./+01  +.90000001./+01  +.90000001./+01
                 +.96000003./+02  +.32000000./+02  +.32000000./+02

+.28475585./-00                   +.11209030./+01  +.16155871./-27
+.28475585./-00                   +.16155871./-27  +.11209030./+01
```

M. I. T. DIGITAL

COMPUTER LAB.

23 Mar.
all Data
#1

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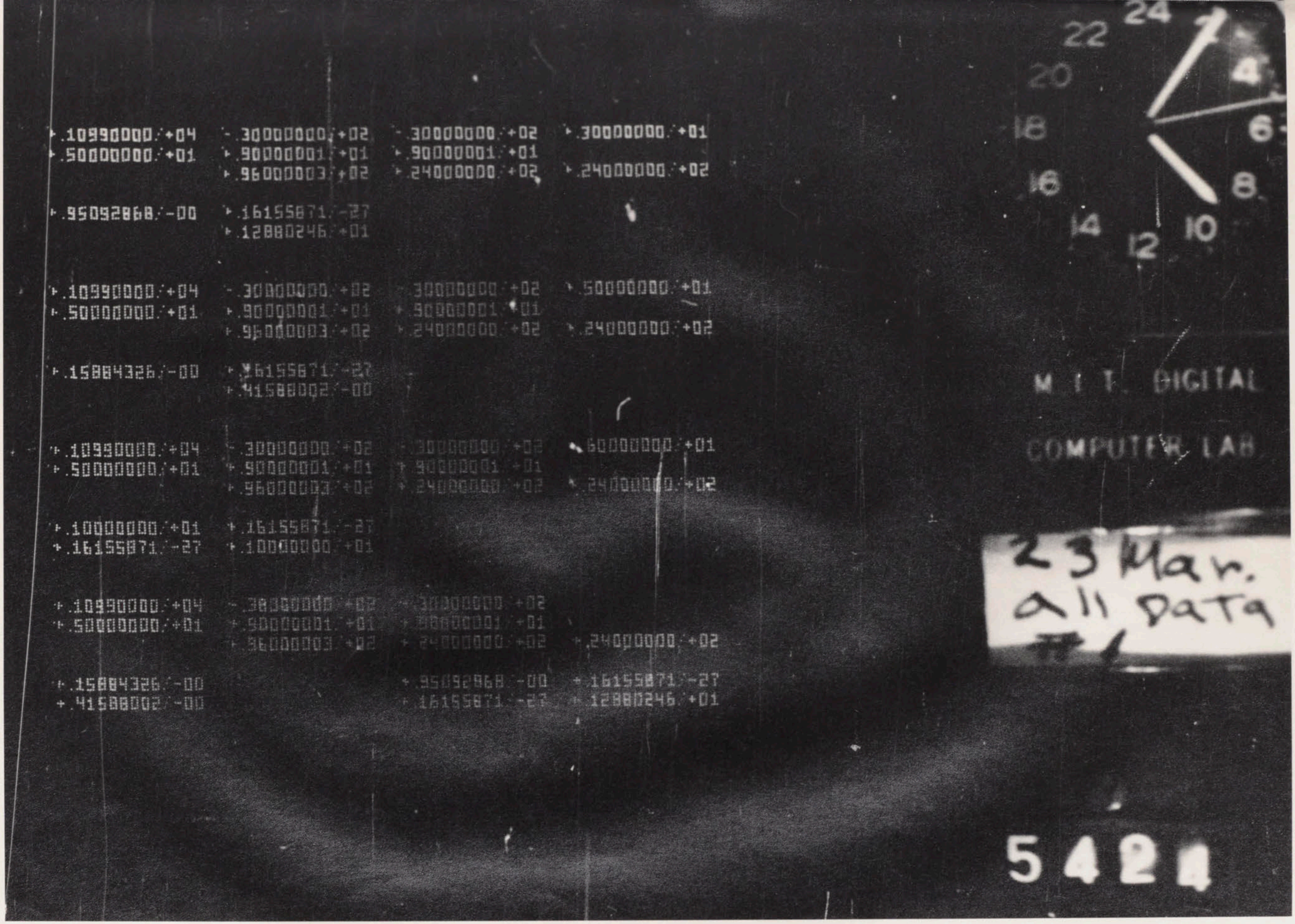


```
+.10990000/+04   -.30000000/+02   -.30000000/+02   +.30000000/+01
+.50000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.24000000/+02   +.24000000/+02

+.95092868/-00   +.16155871/-27
                 +.12880246/+01


+.10990000/+04   -.30000000/+02   -.30000000/+02   +.50000000/+01
+.50000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.24000000/+02   +.24000000/+02

+.15884326/-00   +.16155871/-27
                 +.41588002/-00

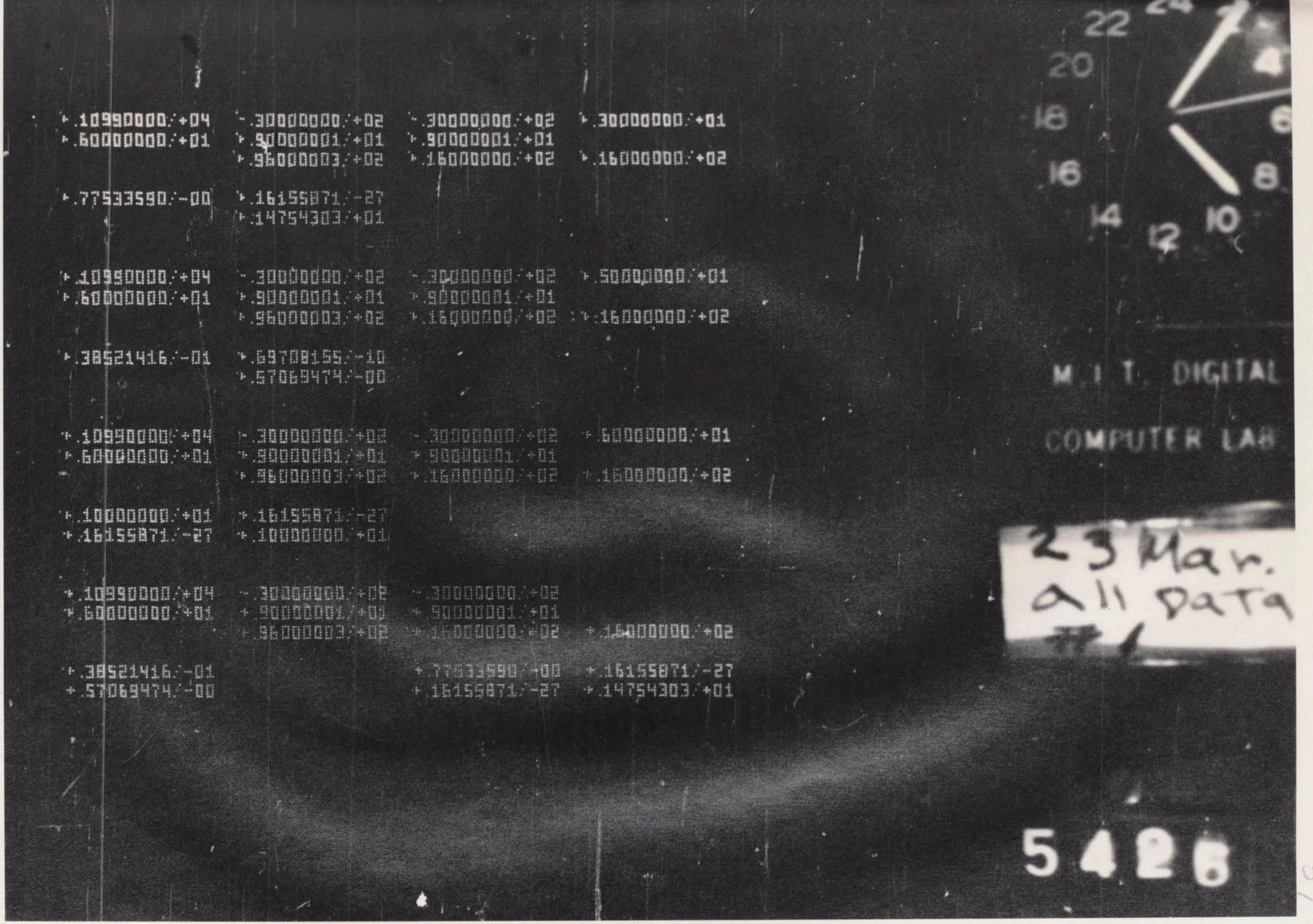

+.10990000/+04   -.30000000/+02   -.30000000/+02   +.60000000/+01
+.50000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.24000000/+02   +.24000000/+02

+.10000000/+01   +.16155871/-27
+.16155871/-27   +.10000000/+01


+.10990000/+04   -.30000000/+02   -.30000000/+02
+.50000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.24000000/+02   +.24000000/+02

+.15884326/-00                    +.95092868/-00   +.16155871/-27
+.41588002/-00                    +.16155871/-27   +.12880246/+01
```

23 Mar.
all Data
#1



```
+.10990000/+04   -.30000000/+02   -.30000000/+02   +.30000000/+01
+.60000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.16000000/+02   +.16000000/+02

+.77533590/-00   +.16155871/-27
                 +.14754303/+01


+.10990000/+04   -.30000000/+02   -.30000000/+02   +.50000000/+01
+.60000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.16000000/+02   +.16000000/+02

+.38521416/-01   +.69708155/-10
                 +.57069474/-00


+.10990000/+04   -.30000000/+02   -.30000000/+02   +.60000000/+01
+.60000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.16000000/+02   +.16000000/+02

+.10000000/+01   +.16155871/-27
+.16155871/-27   +.10000000/+01

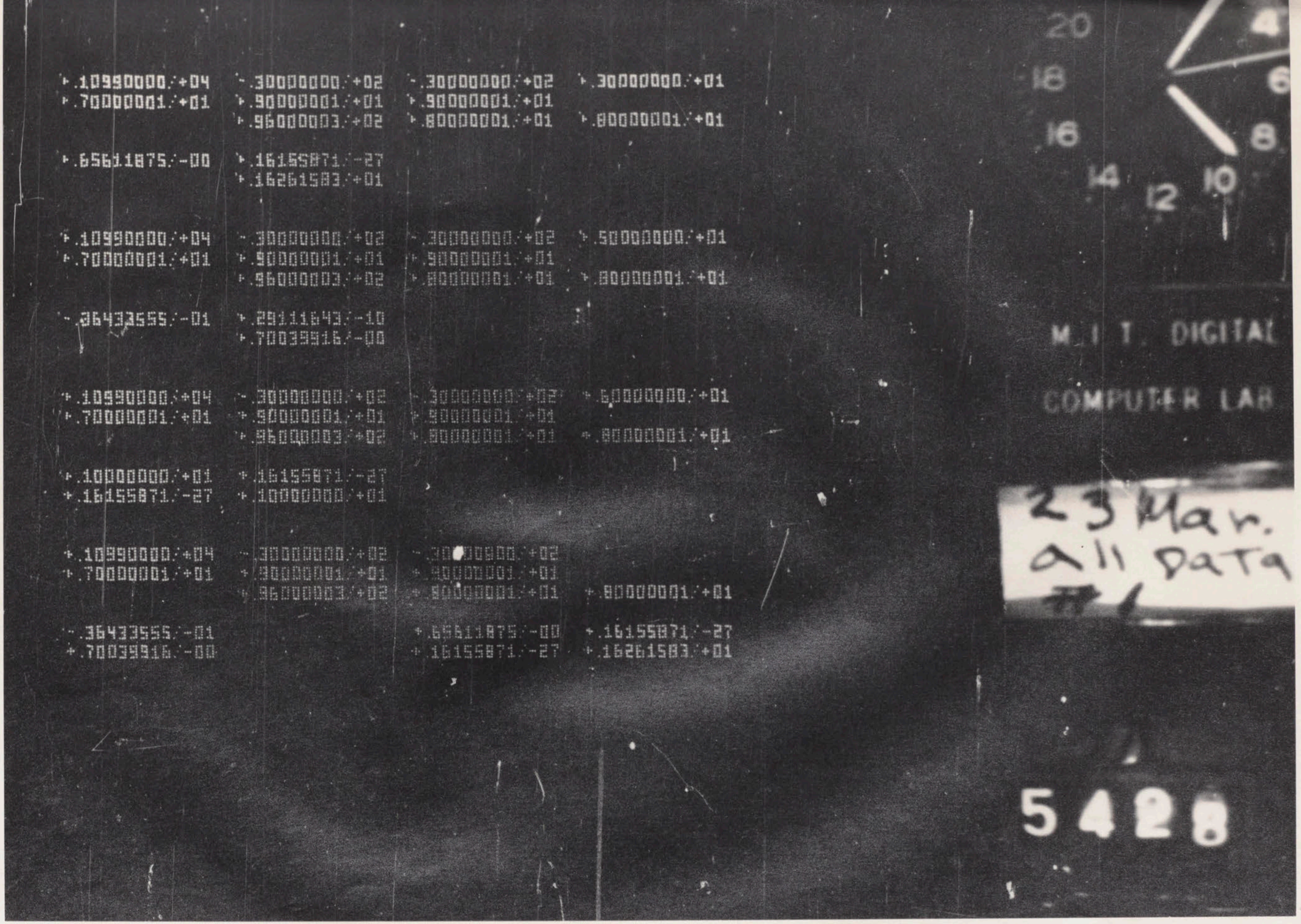

+.10990000/+04   -.30000000/+02   -.30000000/+02
+.60000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.16000000/+02   +.16000000/+02

+.38521416/-01                    +.77533590/-00   +.16155871/-27
+.57069474/-00                    +.16155871/-27   +.14754303/+01
```

M.I.T. DIGITAL
COMPUTER LAB

23 Mar.
all Data
#1

5426



```
+.10990000/+04  -.30000000/+02  -.30000000/+02  +.30000000/+01
+.70000001/+01  +.90000001/+01  +.90000001/+01
                +.96000003/+02  +.80000001/+01  +.80000001/+01

+.65611875/-00  +.16155871/-27
                +.16261583/+01


+.10990000/+04  -.30000000/+02  -.30000000/+02  +.50000000/+01
+.70000001/+01  +.90000001/+01  +.90000001/+01
                +.96000003/+02  +.80000001/+01  +.80000001/+01

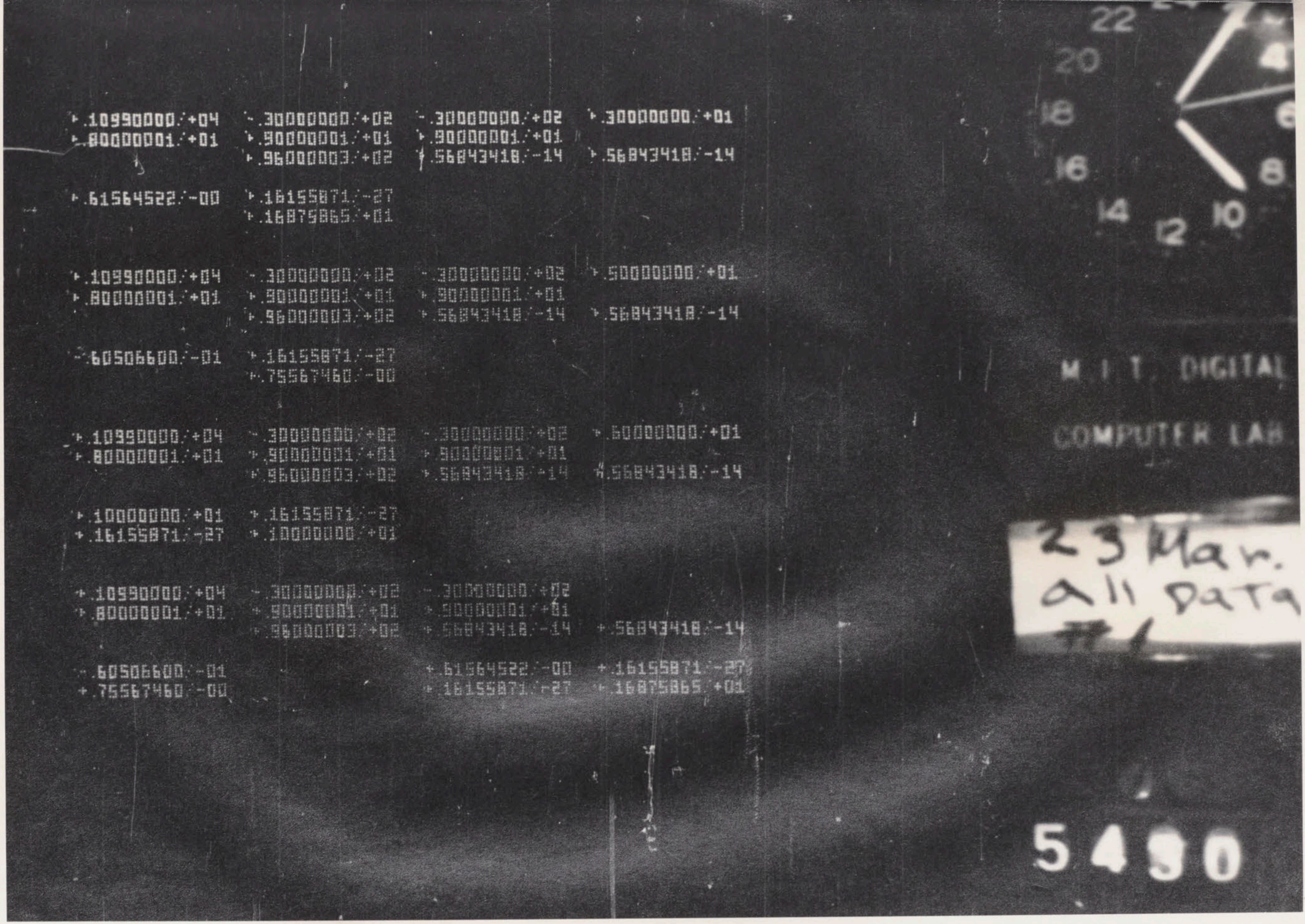
-.36433555/-01  +.29111643/-10
                +.70039916/-00


+.10990000/+04  -.30000000/+02  -.30000000/+02  +.60000000/+01
+.70000001/+01  +.90000001/+01  +.90000001/+01
                +.96000003/+02  +.80000001/+01  +.80000001/+01

+.10000000/+01  +.16155871/-27
+.16155871/-27  +.10000000/+01


+.10990000/+04  -.30000000/+02  -.30000000/+02
+.70000001/+01  +.90000001/+01  +.90000001/+01
                +.96000003/+02  +.80000001/+01  +.80000001/+01

-.36433555/-01                  +.65611875/-00  +.16155871/-27
+.70039916/-00                  +.16155871/-27  +.16261583/+01
```



```
+.10990000/+04   -.30000000/+02   -.30000000/+02   +.30000000/+01
+.80000001/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.56843418/-14   +.56843418/-14

+.61564522/-00   +.16155871/-27
                 +.16875865/+01


+.10990000/+04   -.30000000/+02   -.30000000/+02   +.50000000/+01
+.80000001/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.56843418/-14   +.56843418/-14

-.60506600/-01   +.16155871/-27
                 +.75567460/-00


+.10990000/+04   -.30000000/+02   -.30000000/+02   +.60000000/+01
+.80000001/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.56843418/-14   +.56843418/-14

+.10000000/+01   +.16155871/-27
+.16155871/-27   +.10000000/+01


+.10990000/+04   -.30000000/+02   -.30000000/+02
+.80000001/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.56843418/-14   +.56843418/-14

-.60506600/-01                    +.61564522/-00   +.16155871/-27
+.75567460/-00                    +.16155871/-27   +.16875865/+01
```

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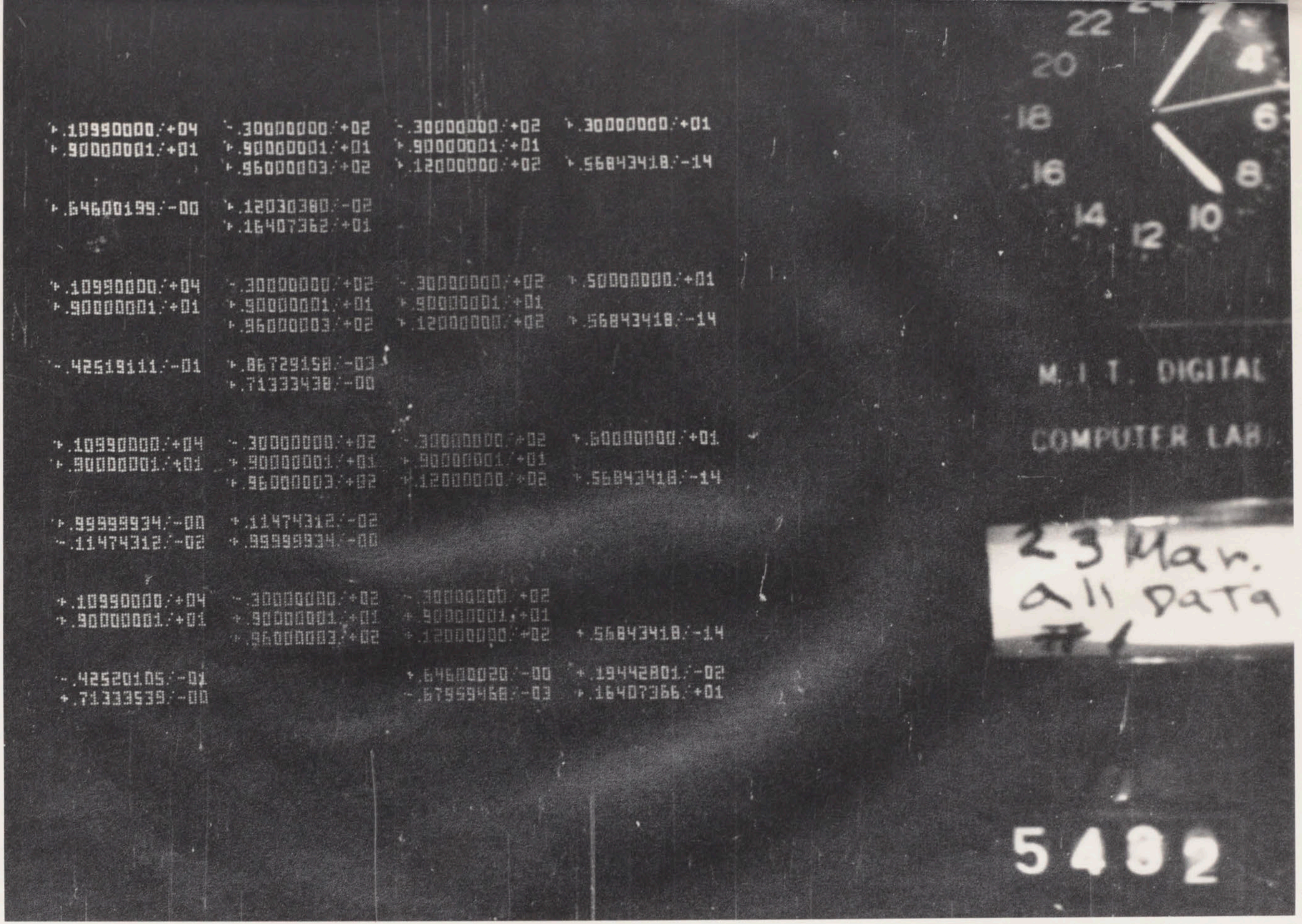
all Data
#1



```
+.10990000/+04   -.30000000/+02   -.30000000/+02   +.30000000/+01
+.90000001/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.12000000/+02   +.56843418/-14

+.64600199/-00   +.12030380/-02
                 +.16407362/+01


+.10990000/+04   -.30000000/+02   -.30000000/+02   +.50000000/+01
+.90000001/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.12000000/+02   +.56843418/-14

-.42519111/-01   +.86729158/-03
                 +.71333438/-00

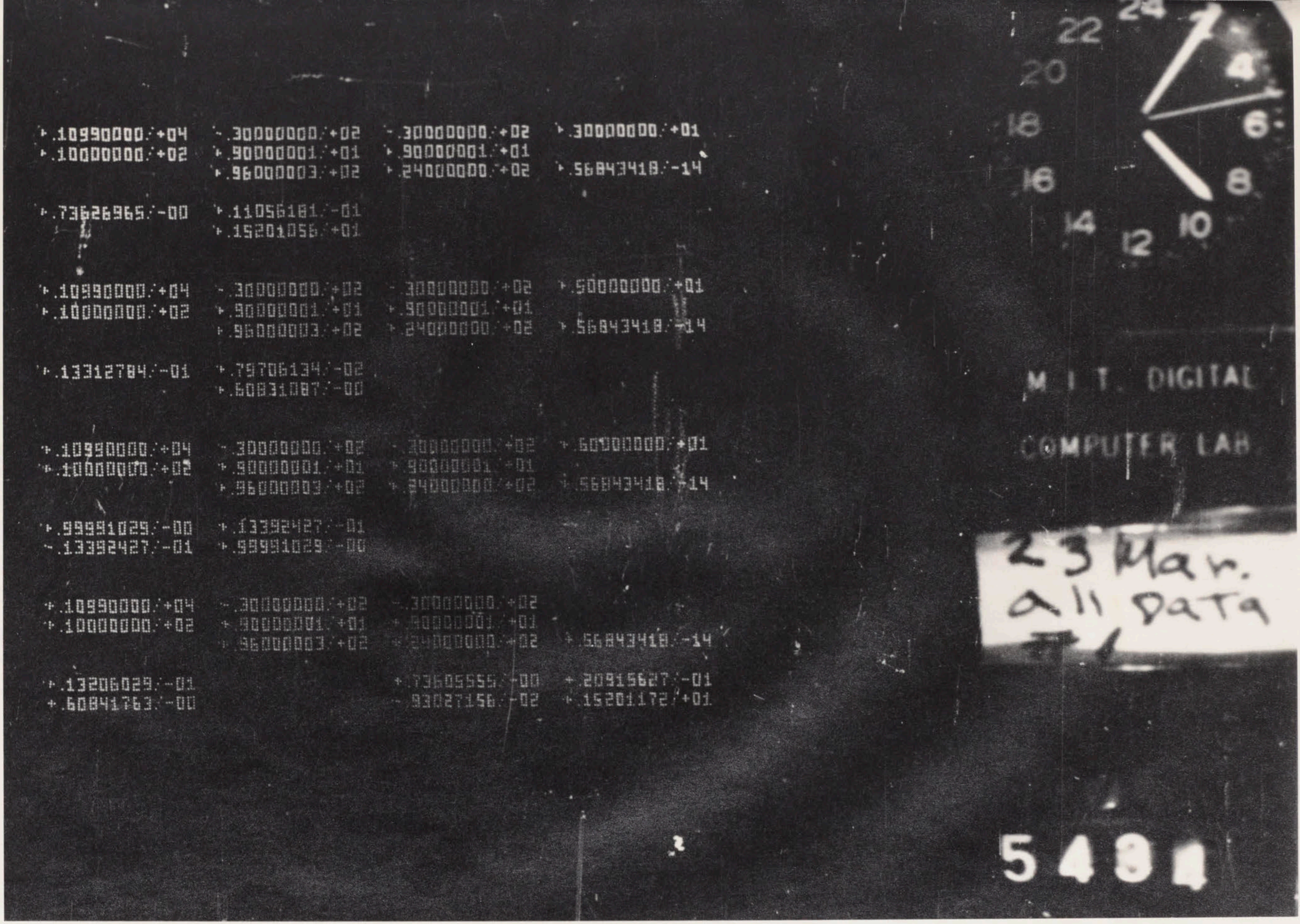

+.10990000/+04   -.30000000/+02   -.30000000/+02   +.60000000/+01
+.90000001/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.12000000/+02   +.56843418/-14

+.99999934/-00   +.11474312/-02
-.11474312/-02   +.99999934/-00


+.10990000/+04   -.30000000/+02   -.30000000/+02
+.90000001/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.12000000/+02   +.56843418/-14

-.42520105/-01                    +.64600020/-00   +.19442801/-02
+.71333539/-00                    -.67959468/-03   +.16407366/+01
```

23 Mar.
all Data
#1



```
+.10990000/+04   -.30000000/+02   -.30000000/+02   +.30000000/+01
+.10000000/+02   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.24000000/+02   +.56843418/-14

+.73626965/-00   +.11056181/-01
                 +.15201056/+01

+.10990000/+04   -.30000000/+02   -.30000000/+02   +.50000000/+01
+.10000000/+02   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.24000000/+02   +.56843418/-14

+.13312784/-01   +.79706134/-02
                 +.60831087/-00

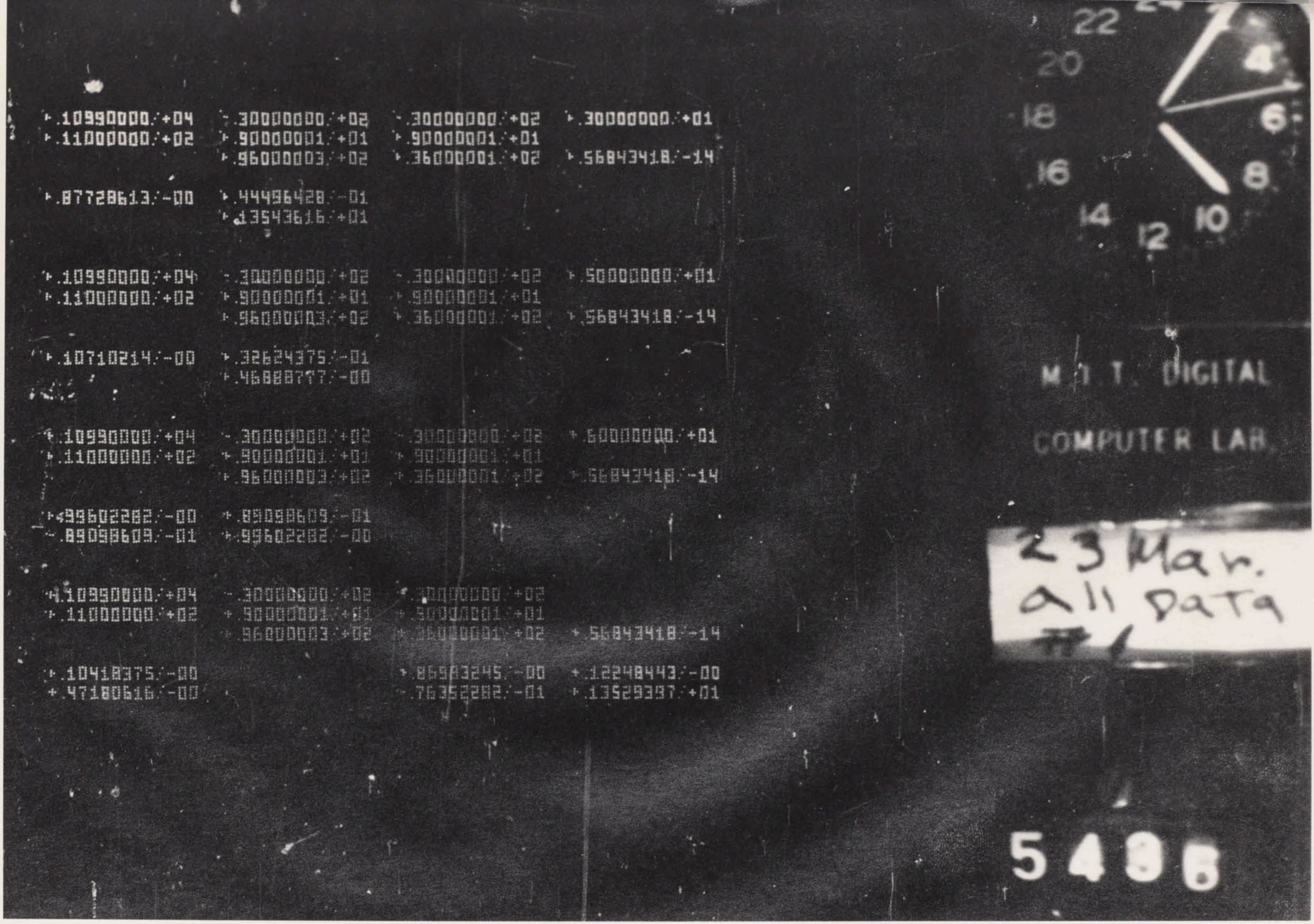
+.10990000/+04   -.30000000/+02   -.30000000/+02   +.60000000/+01
+.10000000/+02   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.24000000/+02   +.56843418/-14

+.99991029/-00   +.13392427/-01
-.13392427/-01   +.99991029/-00

+.10990000/+04   -.30000000/+02   -.30000000/+02
+.10000000/+02   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.24000000/+02   +.56843418/-14

+.13206029/-01                    +.73605555/-00   +.20915627/-01
+.60841763/-00                    -.93027156/-02   +.15201172/+01
```

23 Mar.
all Data
#1



```
+.10990000/+04   -.30000000/+02   -.30000000/+02   +.30000000/+01
+.11000000/+02   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.36000001/+02   +.56843418/-14

+.87728613/-00   +.44496428/-01
                 +.13543616/+01


+.10990000/+04   -.30000000/+02   -.30000000/+02   +.50000000/+01
+.11000000/+02   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.36000001/+02   +.56843418/-14

+.10710214/-00   +.32624375/-01
                 +.46888777/-00


+.10990000/+04   -.30000000/+02   -.30000000/+02   +.60000000/+01
+.11000000/+02   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.36000001/+02   +.56843418/-14

+.99602282/-00   +.89098609/-01
-.89098609/-01   +.99602282/-00


+.10990000/+04   -.30000000/+02    .30000000/+02
+.11000000/+02   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.36000001/+02   +.56843418/-14

+.10418375/-00                    +.86983245/-00   +.12248443/-00
+.47180616/-00                    -.76352282/-01   +.13529397/+01
```

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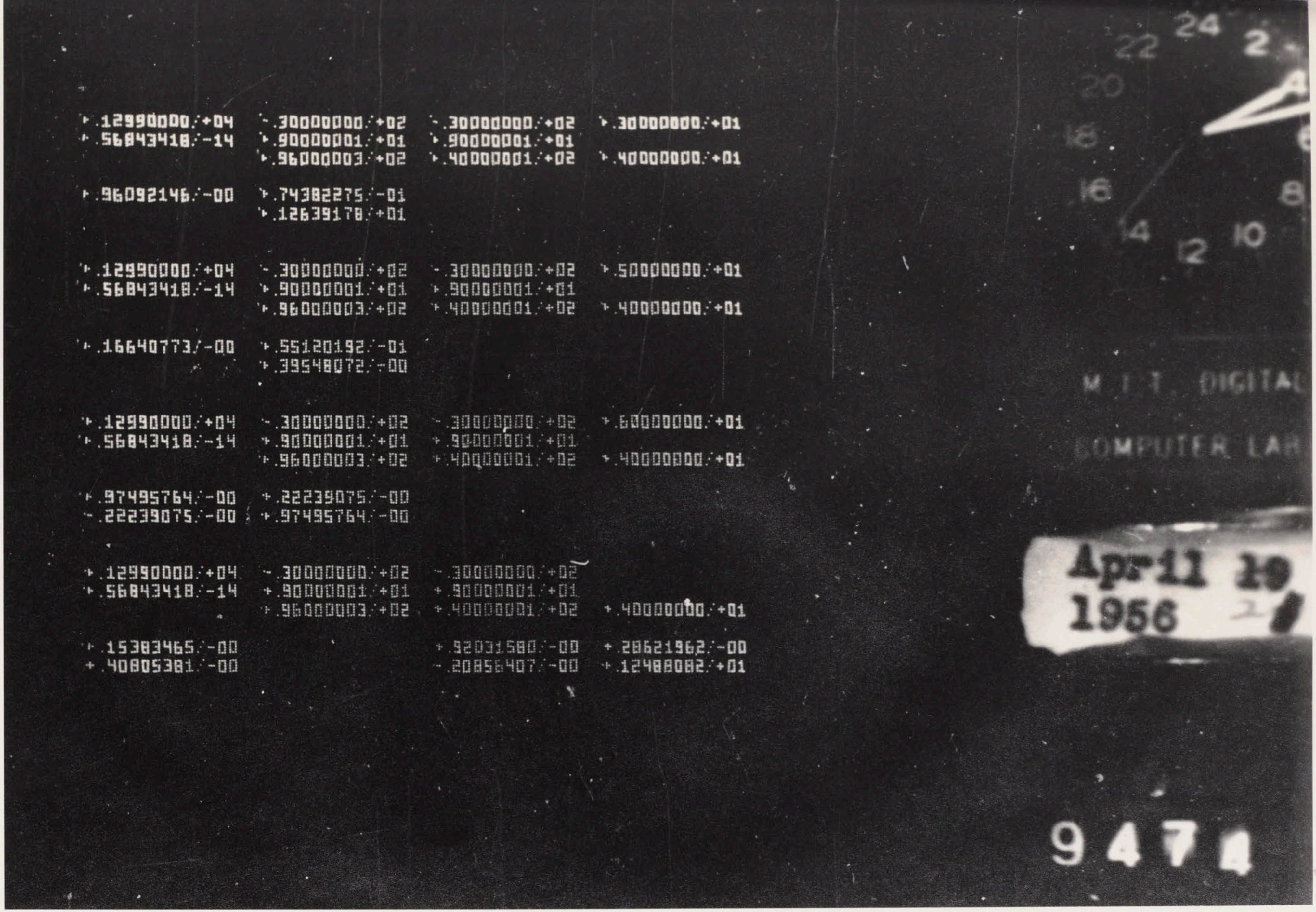


```
+.12990000/+04   -.30000000/+02   -.30000000/+02   +.30000000/+01
+.56843418/-14   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.40000001/+02   +.40000000/+01

+.96092146/-00   +.74382275/-01
                 +.12639178/+01


+.12990000/+04   -.30000000/+02   -.30000000/+02   +.50000000/+01
+.56843418/-14   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.40000001/+02   +.40000000/+01

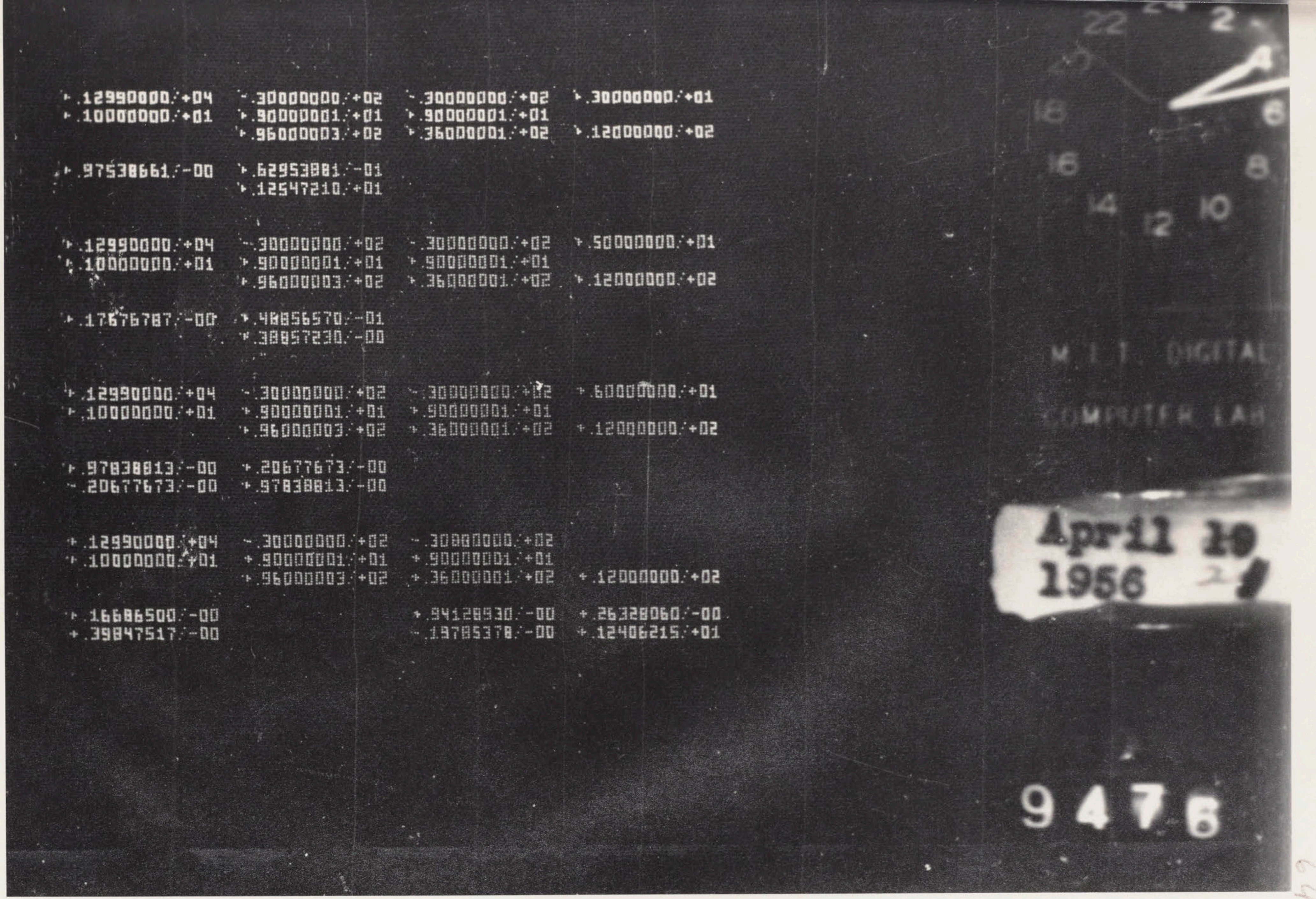
+.16640773/-00   +.55120192/-01
                 +.39548072/-00


+.12990000/+04   -.30000000/+02   -.30000000/+02   +.60000000/+01
+.56843418/-14   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.40000001/+02   +.40000000/+01

+.97495764/-00   +.22239075/-00
-.22239075/-00   +.97495764/-00


+.12990000/+04   -.30000000/+02   -.30000000/+02
+.56843418/-14   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.40000001/+02   +.40000000/+01

+.15383465/-00                    +.92031580/-00   +.28621962/-00
+.40805381/-00                    -.20856407/-00   +.12488082/+01
```



```
+.12990000./+04  -.30000000./+02  -.30000000./+02  +.30000000./+01
+.10000000./+01  +.90000001./+01  +.90000001./+01
                 +.96000003./+02  +.36000001./+02  +.12000000./+02

+.97538661./-00  +.62953881./-01
                 +.12547210./+01


+.12990000./+04  -.30000000./+02  -.30000000./+02  +.50000000./+01
+.10000000./+01  +.90000001./+01  +.90000001./+01
                 +.96000003./+02  +.36000001./+02  +.12000000./+02

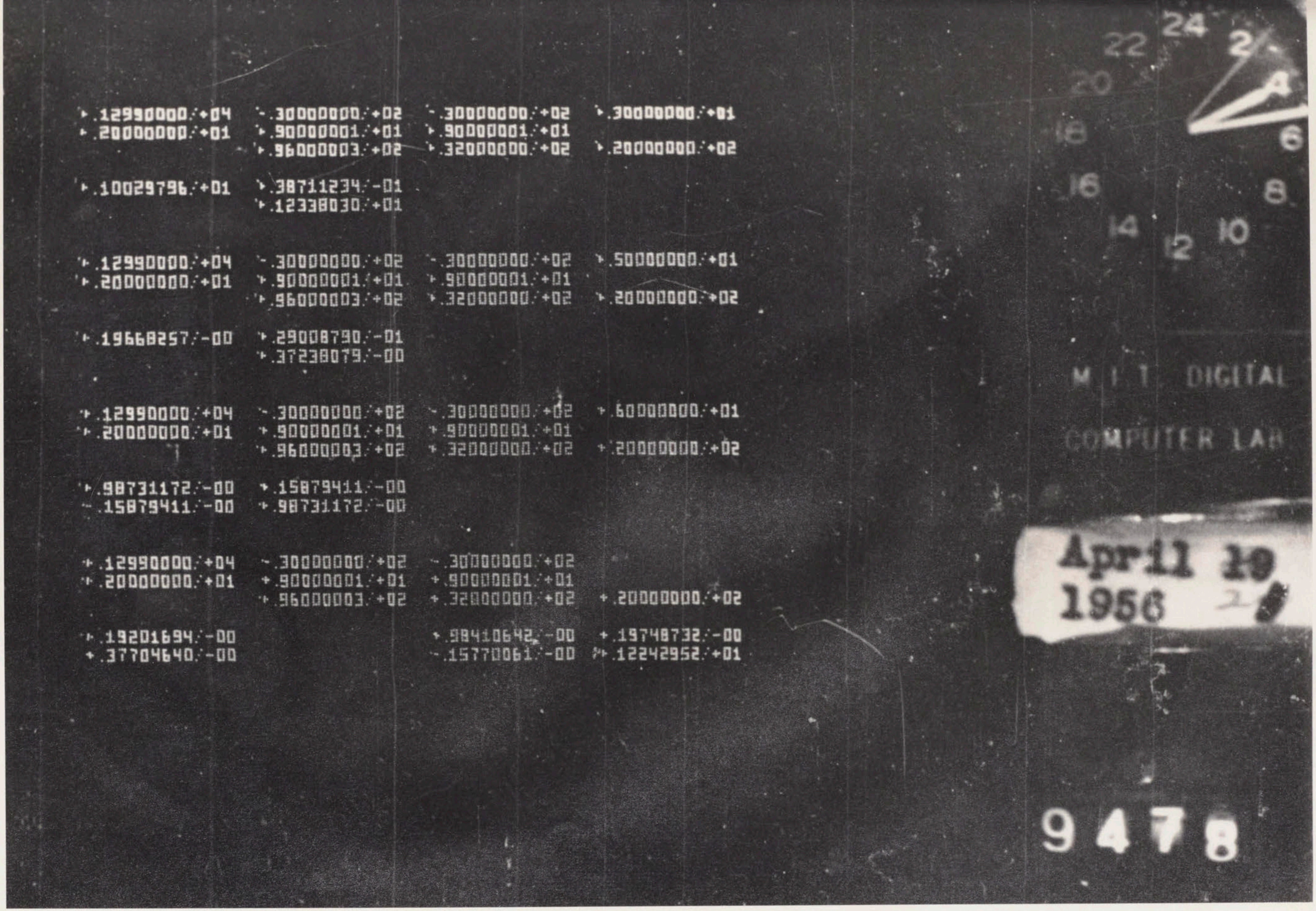
+.17676787./-00  +.40856570./-01
                 +.38857230./-00


+.12990000./+04  -.30000000./+02  -.30000000./+02  +.60000000./+01
+.10000000./+01  +.90000001./+01  +.90000001./+01
                 +.96000003./+02  +.36000001./+02  +.12000000./+02

+.97838813./-00  +.20677673./-00
-.20677673./-00  +.97838813./-00


+.12990000./+04  -.30000000./+02  -.30880000./+02
+.10000000./+01  +.90000001./+01  +.90000001./+01
                 +.96000003./+02  +.36000001./+02  +.12000000./+02

+.16686500./-00                   +.94128930./-00  +.26328060./-00
+.39847517./-00                   -.19785378./-00  +.12406215./+01
```



```
+.12990000./+04   -.30000000./+02   -.30000000./+02   +.30000000./+01
+.20000000./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.32000000./+02   +.20000000./+02

+.10029796./+01   +.38711234./-01
                  +.12338030./+01


+.12990000./+04   -.30000000./+02   -.30000000./+02   +.50000000./+01
+.20000000./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.32000000./+02   +.20000000./+02

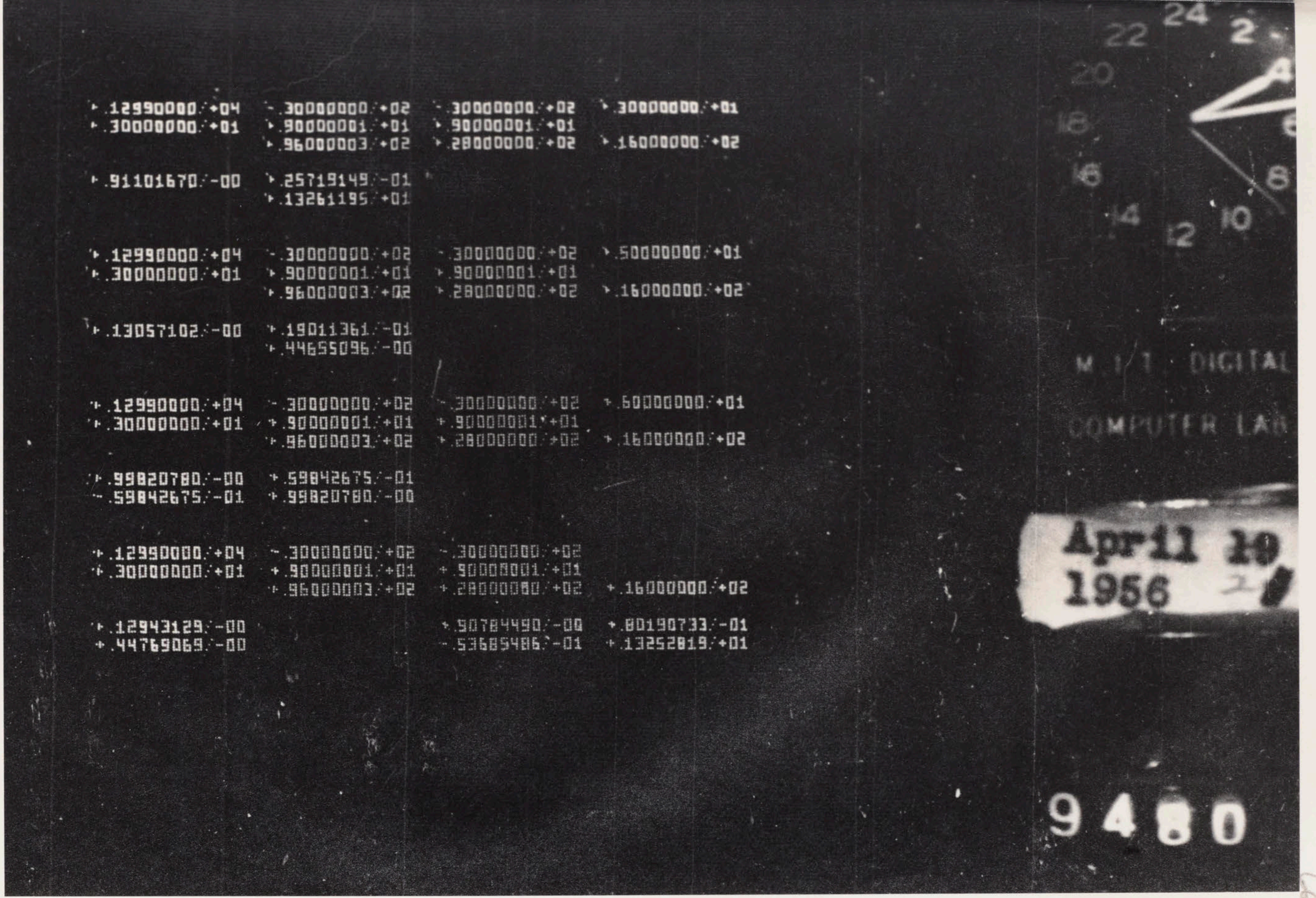
+.19668257./-00   +.29008790./-01
                  +.37238079./-00


+.12990000./+04   -.30000000./+02   -.30000000./+02   +.60000000./+01
+.20000000./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.32000000./+02   +.20000000./+02

+.98731172./-00   +.15879411./-00
-.15879411./-00   +.98731172./-00


+.12990000./+04   -.30000000./+02   -.30000000./+02
+.20000000./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.32000000./+02   +.20000000./+02

+.19201694./-00                     +.98410642./-00   +.19748732./-00
+.37704640./-00                     -.15770061./-00   +.12242952./+01
```



```
+.12990000/+04   -.30000000/+02   -.30000000/+02   +.30000000/+01
+.30000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.28000000/+02   +.16000000/+02

+.91101670/-00   +.25719149/-01
                 +.13261195/+01


+.12990000/+04   -.30000000/+02   -.30000000/+02   +.50000000/+01
+.30000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.28000000/+02   +.16000000/+02

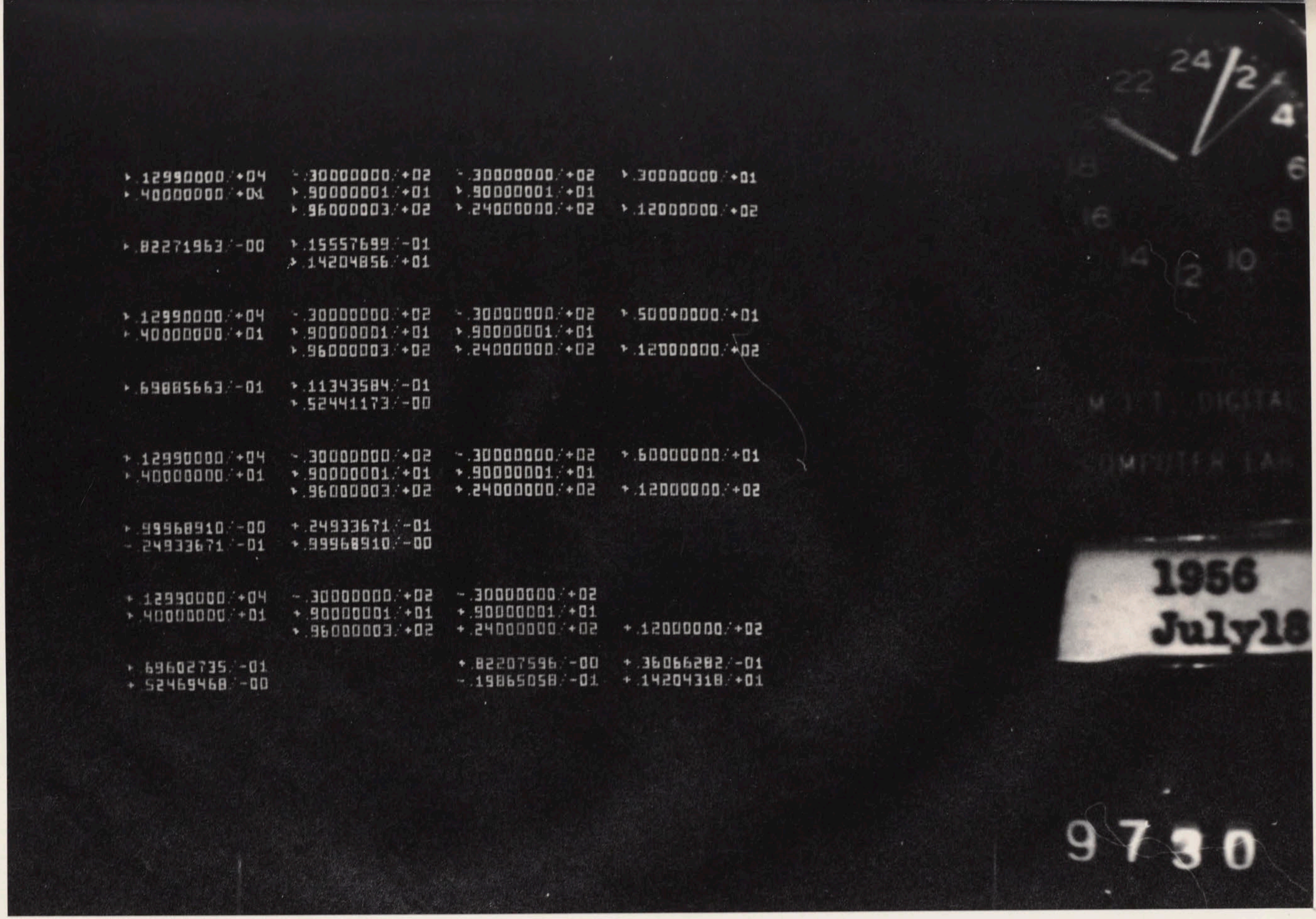
+.13057102/-00   +.19011361/-01
                 +.44655096/-00


+.12990000/+04   -.30000000/+02   -.30000000/+02   +.60000000/+01
+.30000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.28000000/+02   +.16000000/+02

+.99820780/-00   +.59842675/-01
-.59842675/-01   +.99820780/-00


+.12990000/+04   -.30000000/+02   -.30000000/+02
+.30000000/+01   +.90000001/+01   +.90008001/+01
                 +.96000003/+02   +.28000080/+02   +.16000000/+02

+.12943129/-00                    +.90784490/-00   +.80190733/-01
+.44769069/-00                    -.53685486/-01   +.13252819/+01
```



```
+.12990000/+04   -.30000000/+02   -.30000000/+02   +.30000000/+01
+.40000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.24000000/+02   +.12000000/+02

+.82271963/-00   +.15557699/-01
                 +.14204856/+01


+.12990000/+04   -.30000000/+02   -.30000000/+02   +.50000000/+01
+.40000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.24000000/+02   +.12000000/+02

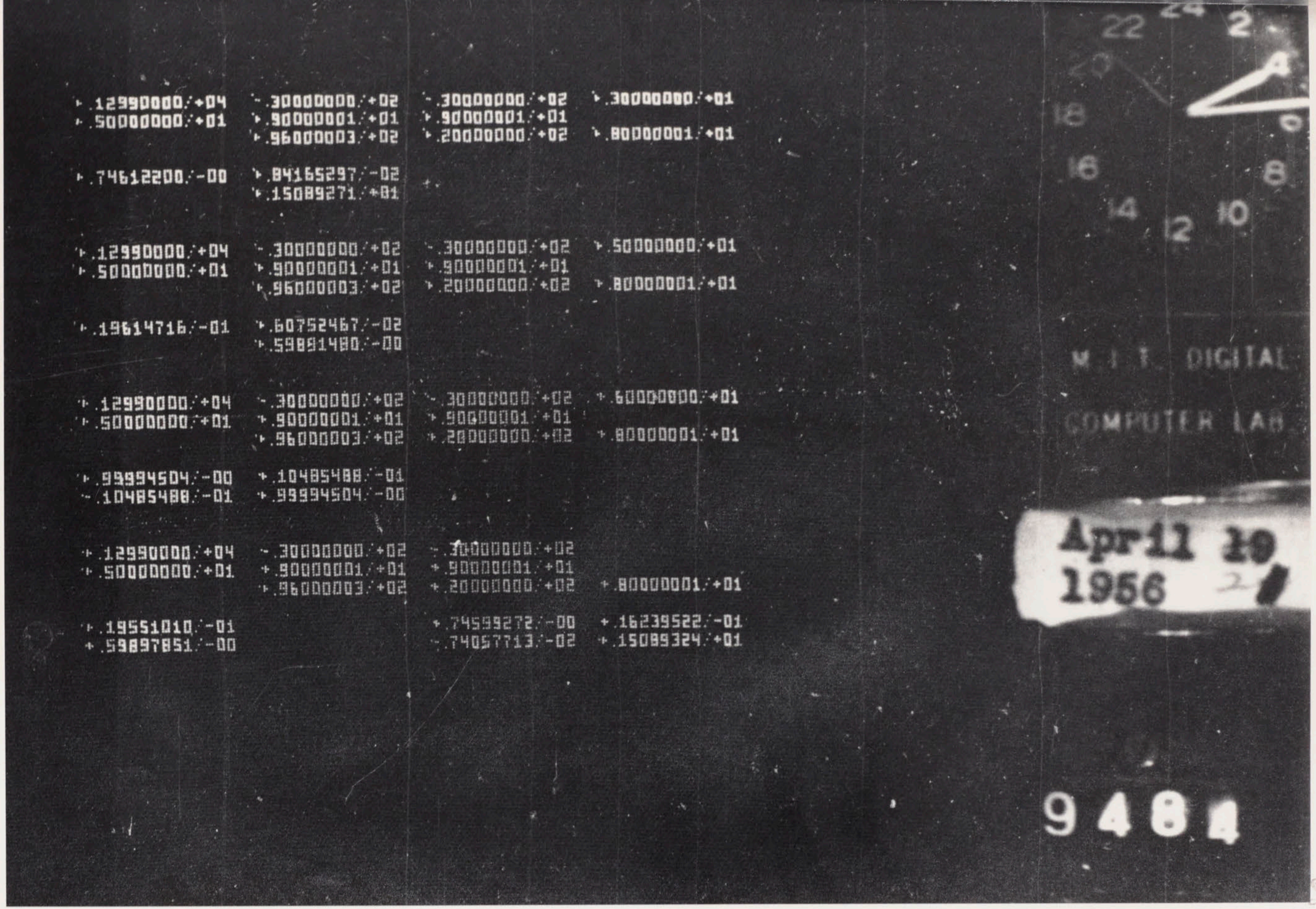
+.69885663/-01   +.11343584/-01
                 +.52441173/-00


+.12990000/+04   -.30000000/+02   -.30000000/+02   +.60000000/+01
+.40000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.24000000/+02   +.12000000/+02

+.99968910/-00   +.24933671/-01
-.24933671/-01   +.99968910/-00


+.12990000/+04   -.30000000/+02   -.30000000/+02
+.40000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.24000000/+02   +.12000000/+02

+.69602735/-01                    +.82207596/-00   +.36066282/-01
+.52469468/-00                    -.19865058/-01   +.14204318/+01
```



```
+.12990000./+04   -.30000000./+02   -.30000000./+02   +.30000000./+01
+.50000000./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.20000000./+02   +.80000001./+01

+.74612200./-00   +.84165297./-02
                  +.15089271./+01

+.12990000./+04   -.30000000./+02   -.30000000./+02   +.50000000./+01
+.50000000./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.20000000./+02   +.80000001./+01

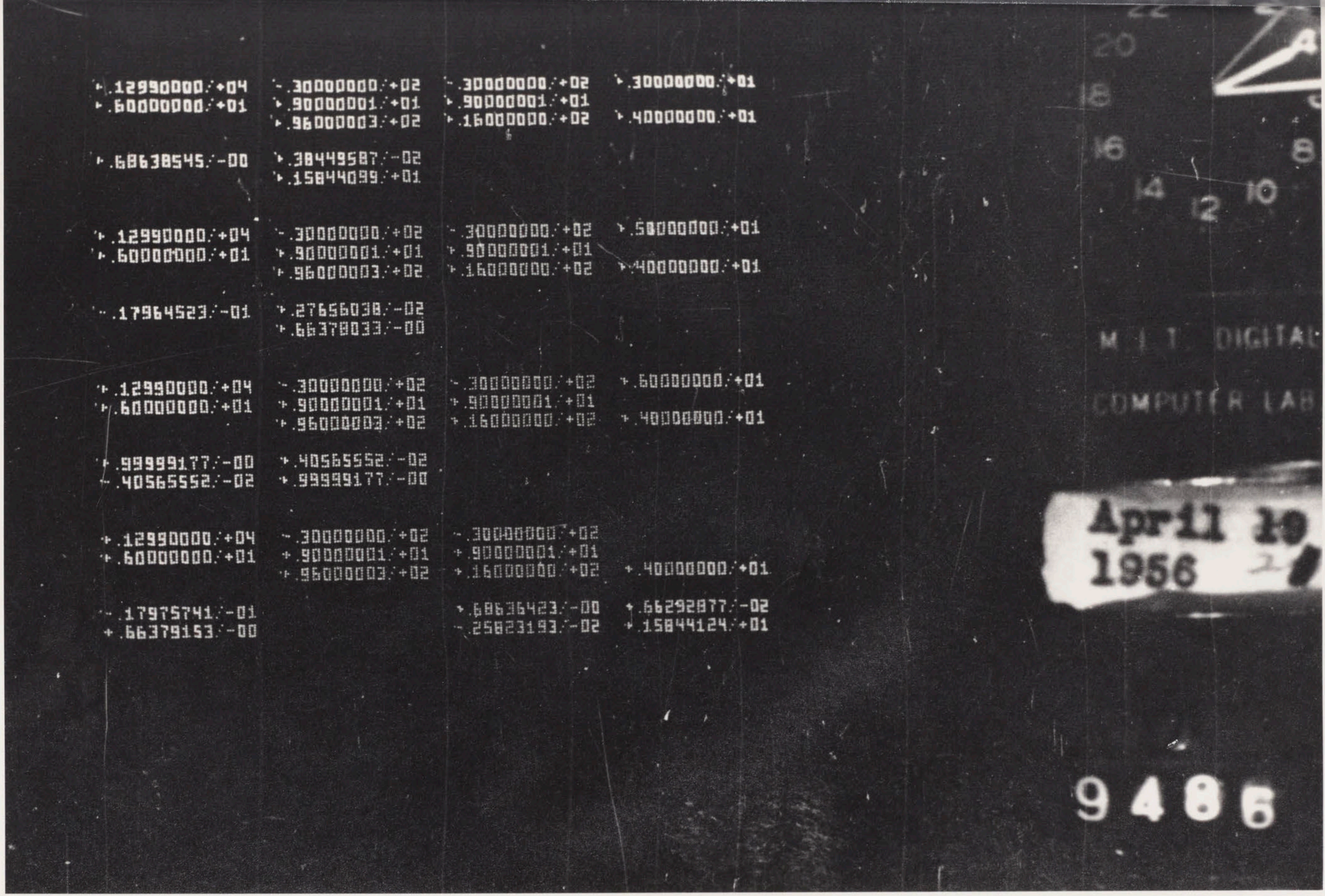
+.19614716./-01   +.60752467./-02
                  +.59891480./-00

+.12990000./+04   -.30000000./+02   -.30000000./+02   +.60000000./+01
+.50000000./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.20000000./+02   +.80000001./+01

+.99994504./-00   +.10485488./-01
-.10485488./-01   +.99994504./-00

+.12990000./+04   -.30000000./+02   -.30000000./+02
+.50000000./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.20000000./+02   +.80000001./+01

+.19551010./-01                     +.74599272./-00   +.16239522./-01
+.59897851./-00                     -.74057713./-02   +.15089324./+01
```



April 19
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```
+.12990000/+04   -.30000000/+02   -.30000000/+02   +.30000000/+01
+.60000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.16000000/+02   +.40000000/+01

+.68638545/-00   +.38449587/-02
                 +.15844099/+01


+.12990000/+04   -.30000000/+02   -.30000000/+02   +.50000000/+01
+.60000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.16000000/+02   +.40000000/+01

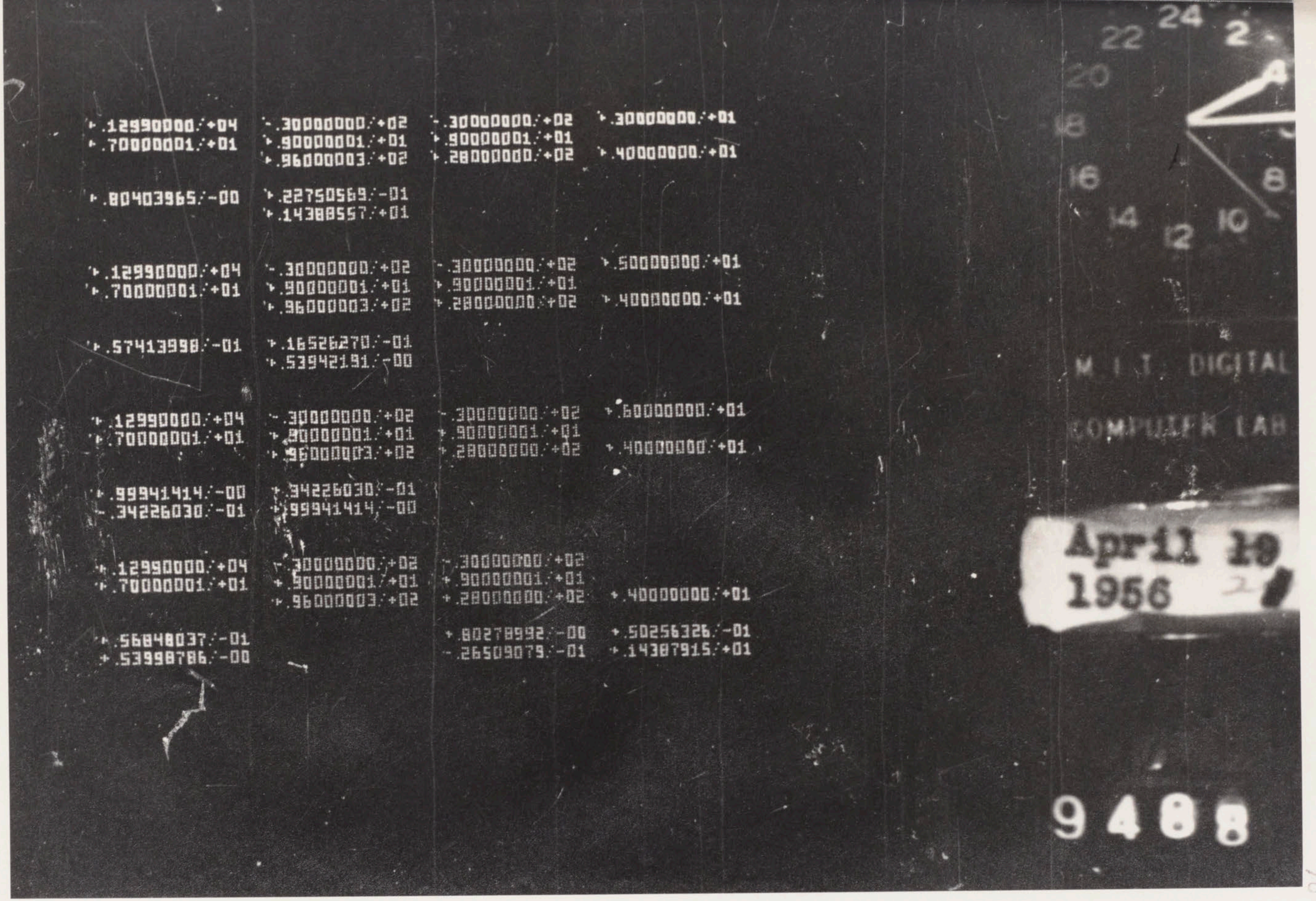
-.17964523/-01   +.27656038/-02
                 +.66378033/-00


+.12990000/+04   -.30000000/+02   -.30000000/+02   +.60000000/+01
+.60000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.16000000/+02   +.40000000/+01

+.99999177/-00   +.40565552/-02
-.40565552/-02   +.99999177/-00


+.12990000/+04   -.30000000/+02   -.30000000/+02
+.60000000/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.16000000/+02   +.40000000/+01

-.17975741/-01                    +.68636423/-00   +.66292877/-02
+.66379153/-00                    -.25823193/-02   +.15844124/+01
```



```
+.12990000./+04   -.30000000./+02   -.30000000./+02   +.30000000./+01
+.70000001./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.28000000./+02   +.40000000./+01

+.80403965./-00   +.22750569./-01
                  +.14388557./+01


+.12990000./+04   -.30000000./+02   -.30000000./+02   +.50000000./+01
+.70000001./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.28000000./+02   +.40000000./+01

+.57413998./-01   +.16526270./-01
                  +.53942191./-00

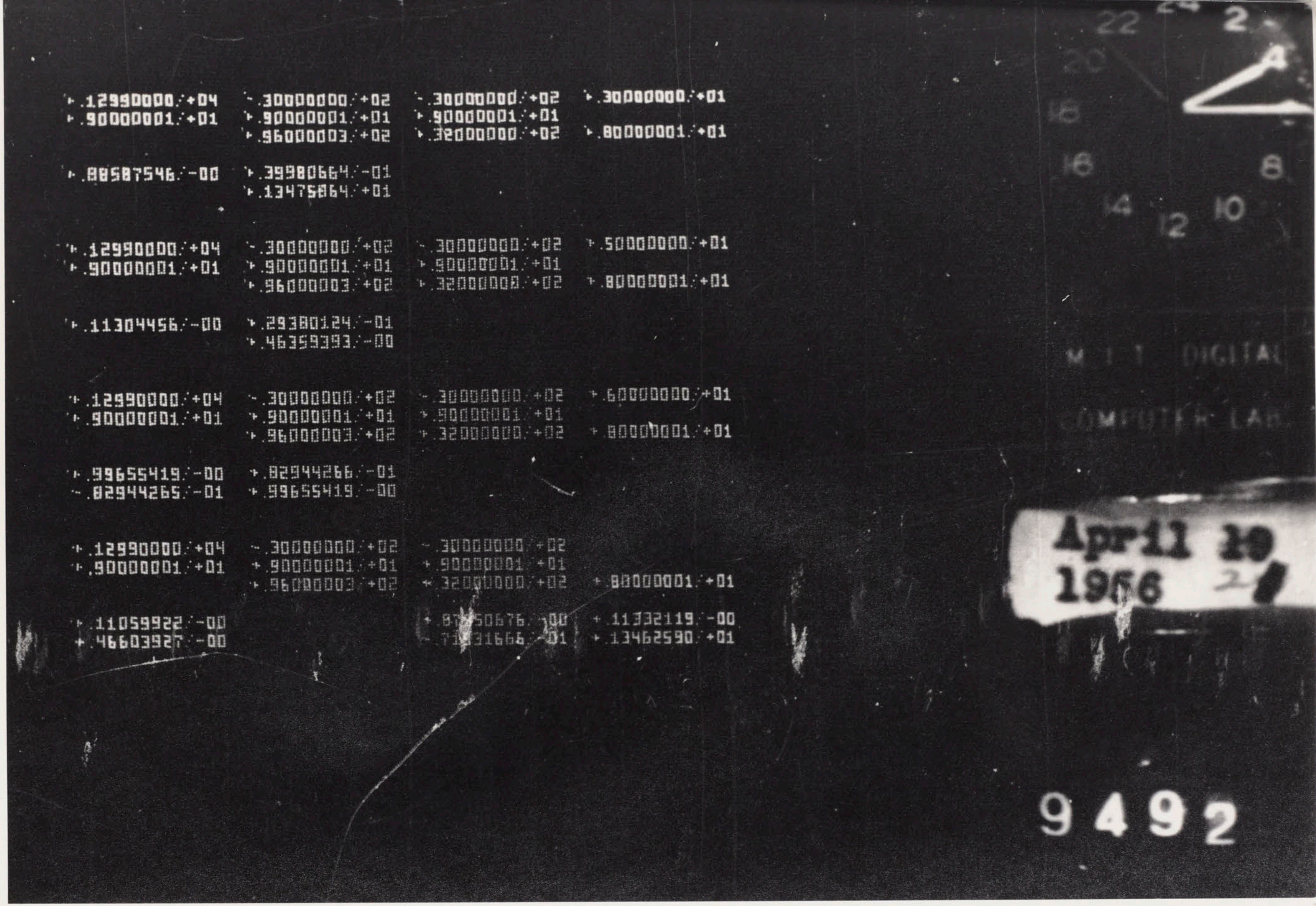

+.12990000./+04   -.30000000./+02   -.30000000./+02   +.60000000./+01
+.70000001./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.28000000./+02   +.40000000./+01

+.99941414./-00   +.34226030./-01
-.34226030./-01   +.99941414./-00


+.12990000./+04   -.30000000./+02   -.30000000./+02
+.70000001./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.28000000./+02   +.40000000./+01

+.56848037./-01                     +.80278992./-00   +.50256326./-01
+.53998786./-00                     -.26509079./-01   +.14387915./+01
```

20



```
+.12990000./+04   -.30000000./+02   -.30000000./+02   +.30000000./+01
+.90000001./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.32000000./+02   +.80000001./+01

+.08587546./-00   +.39980664./-01
                  +.13475864./+01


+.12990000./+04   -.30000000./+02   -.30000000./+02   +.50000000./+01
+.90000001./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.32000000./+02   +.80000001./+01

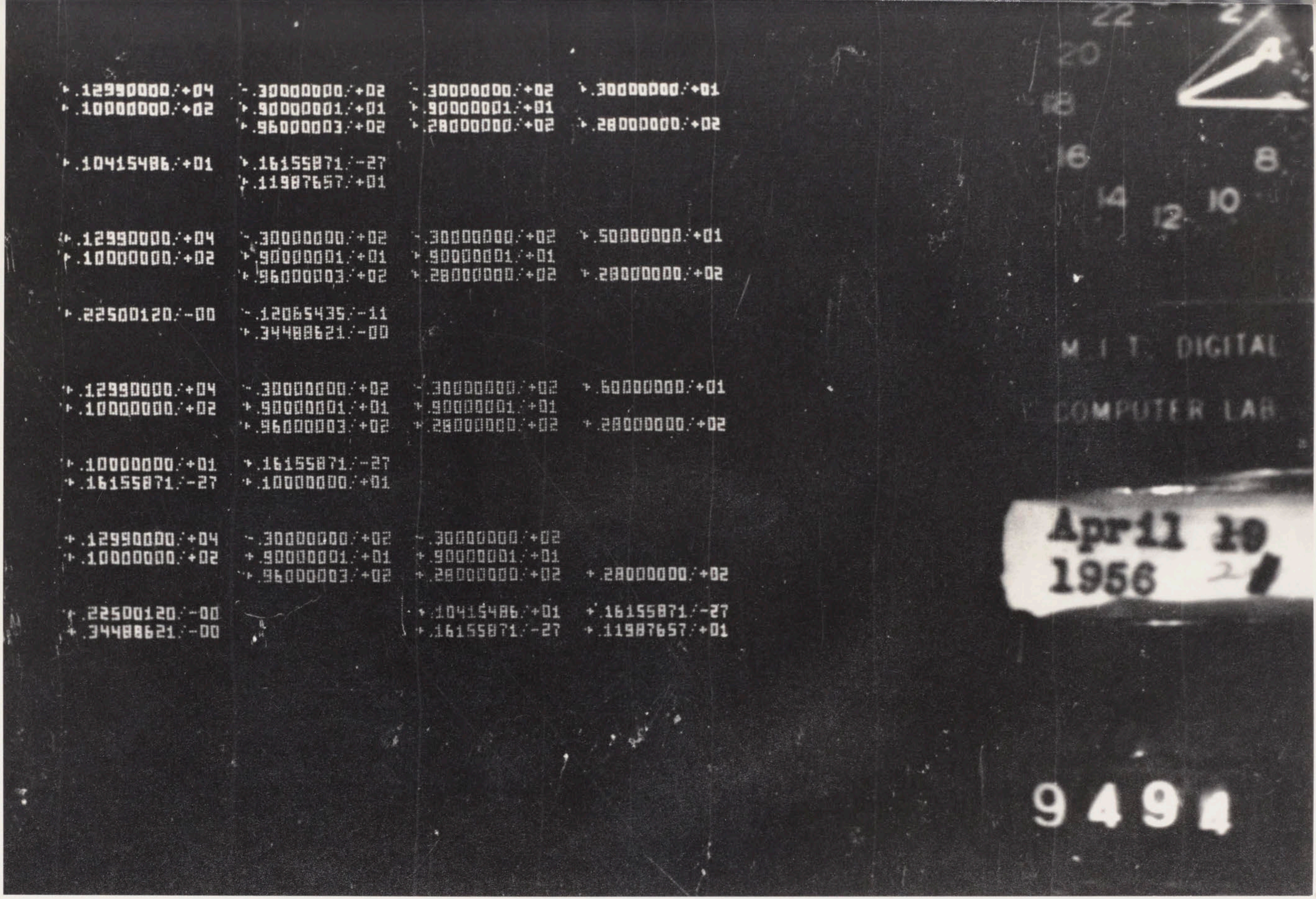
+.11304456./-00   +.29380124./-01
                  +.46359393./-00


+.12990000./+04   -.30000000./+02   -.30000000./+02   +.60000000./+01
+.90000001./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.32000000./+02   +.80000001./+01

+.99655419./-00   +.82944266./-01
-.82944265./-01   +.99655419./-00


+.12990000./+04   -.30000000./+02   -.30000000./+02
+.90000001./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.32000000./+02   +.80000001./+01

+.11059922./-00                     +.87[illegible]50676./-00   +.11332119./-00
+.46603927./-00                     -.71[illegible]31666./-01   +.13462590./+01
```



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+.12990000.+04   -.30000000.+02   -.30000000.+02   +.30000000.+01
+.10000000.+02   +.90000001.+01   +.90000001.+01
                 +.96000003.+02   +.28000000.+02   +.28000000.+02

+.10415486.+01   +.16155871.-27
                 +.11987657.+01


+.12990000.+04   -.30000000.+02   -.30000000.+02   +.50000000.+01
+.10000000.+02   +.90000001.+01   +.90000001.+01
                 +.96000003.+02   +.28000000.+02   +.28000000.+02

+.22500120.-00   -.12065435.-11
                 +.34488621.-00


+.12990000.+04   -.30000000.+02   -.30000000.+02   +.60000000.+01
+.10000000.+02   +.90000001.+01   +.90000001.+01
                 +.96000003.+02   +.28000000.+02   +.28000000.+02

+.10000000.+01   +.16155871.-27
+.16155871.-27   +.10000000.+01


+.12990000.+04   -.30000000.+02   -.30000000.+02
+.10000000.+02   +.90000001.+01   +.90000001.+01
                 +.96000003.+02   +.28000000.+02   +.28000000.+02

+.22500120.-00                    +.10415486.+01   +.16155871.-27
+.34488621.-00                    +.16155871.-27   +.11987657.+01
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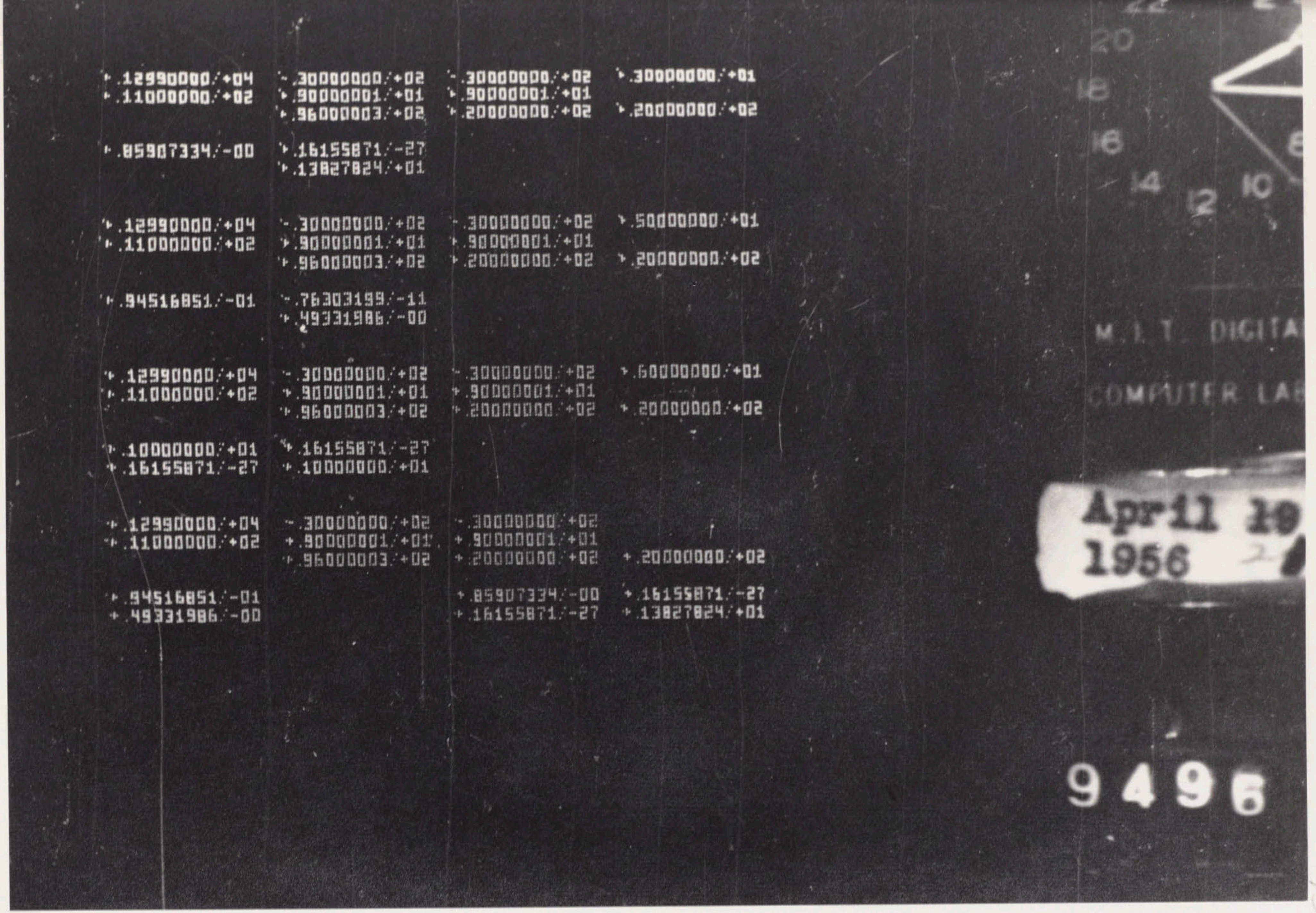


```
+.12990000/+04   -.30000000/+02   -.30000000/+02   +.30000000/+01
+.11000000/+02   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.20000000/+02   +.20000000/+02

+.85907334/-00   +.16155871/-27
                 +.13827824/+01


+.12990000/+04   -.30000000/+02   -.30000000/+02   +.50000000/+01
+.11000000/+02   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.20000000/+02   +.20000000/+02

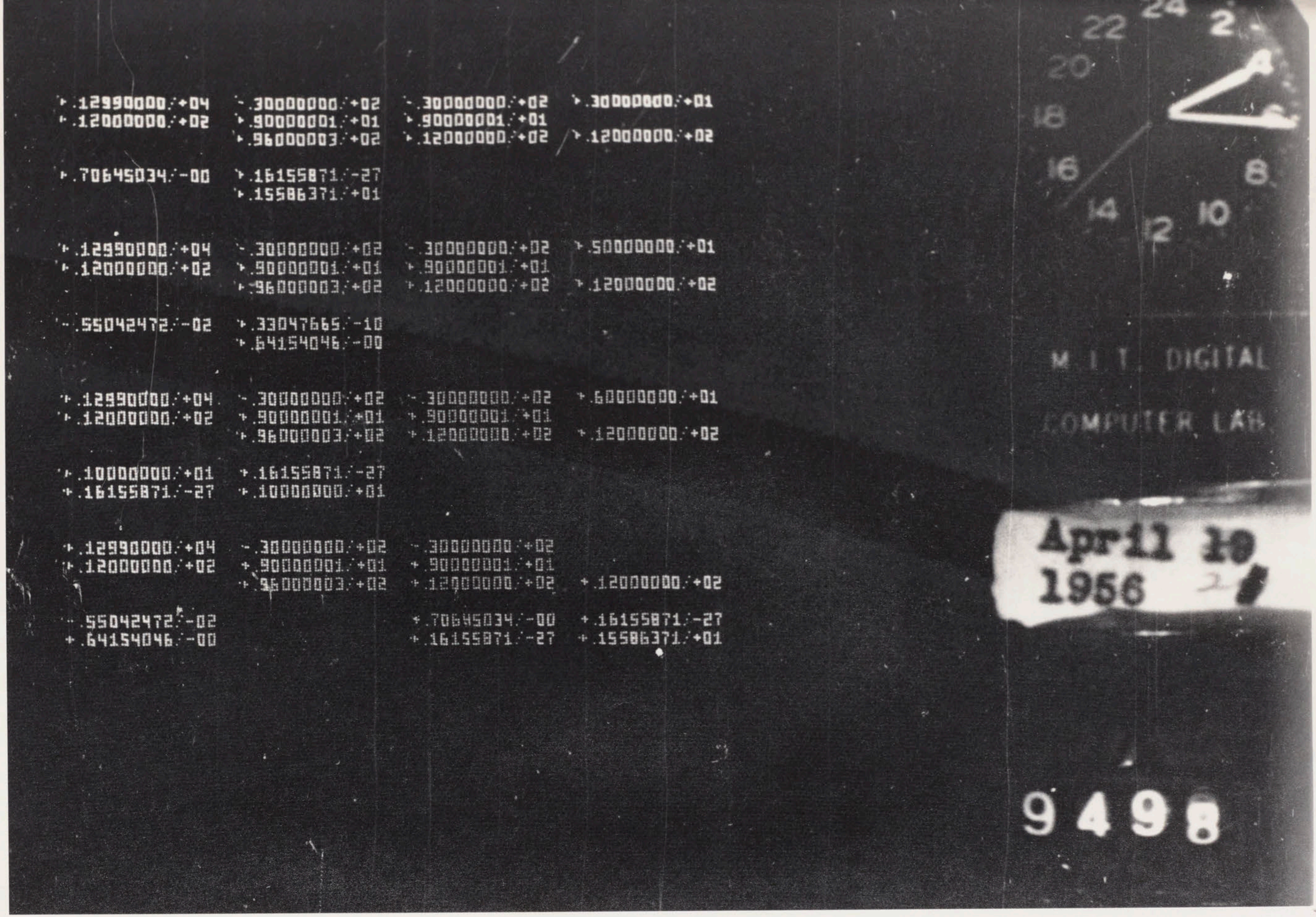
+.94516851/-01   -.76303199/-11
                 +.49331986/-00


+.12990000/+04   -.30000000/+02   -.30000000/+02   +.60000000/+01
+.11000000/+02   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.20000000/+02   +.20000000/+02

+.10000000/+01   +.16155871/-27
+.16155871/-27   +.10000000/+01


+.12990000/+04   -.30000000/+02   -.30000000/+02
+.11000000/+02   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.20000000/+02   +.20000000/+02

+.94516851/-01                    +.85907334/-00   +.16155871/-27
+.49331986/-00                    +.16155871/-27   +.13827824/+01
```



```
+.12990000./+04   -.30000000./+02   -.30000000./+02   +.30000000./+01
+.12000000./+02   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.12000000./+02   +.12000000./+02

+.70645034./-00   +.16155871./-27
                  +.15586371./+01


+.12990000./+04   -.30000000./+02   -.30000000./+02   +.50000000./+01
+.12000000./+02   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.12000000./+02   +.12000000./+02

-.55042472./-02   +.33047665./-10
                  +.64154046./-00


+.12990000./+04   -.30000000./+02   -.30000000./+02   +.60000000./+01
+.12000000./+02   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.12000000./+02   +.12000000./+02

+.10000000./+01   +.16155871./-27
+.16155871./-27   +.10000000./+01


+.12990000./+04   -.30000000./+02   -.30000000./+02
+.12000000./+02   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.12000000./+02   +.12000000./+02

-.55042472./-02                     +.70645034./-00   +.16155871./-27
+.64154046./-00                     +.16155871./-27   +.15586371./+01
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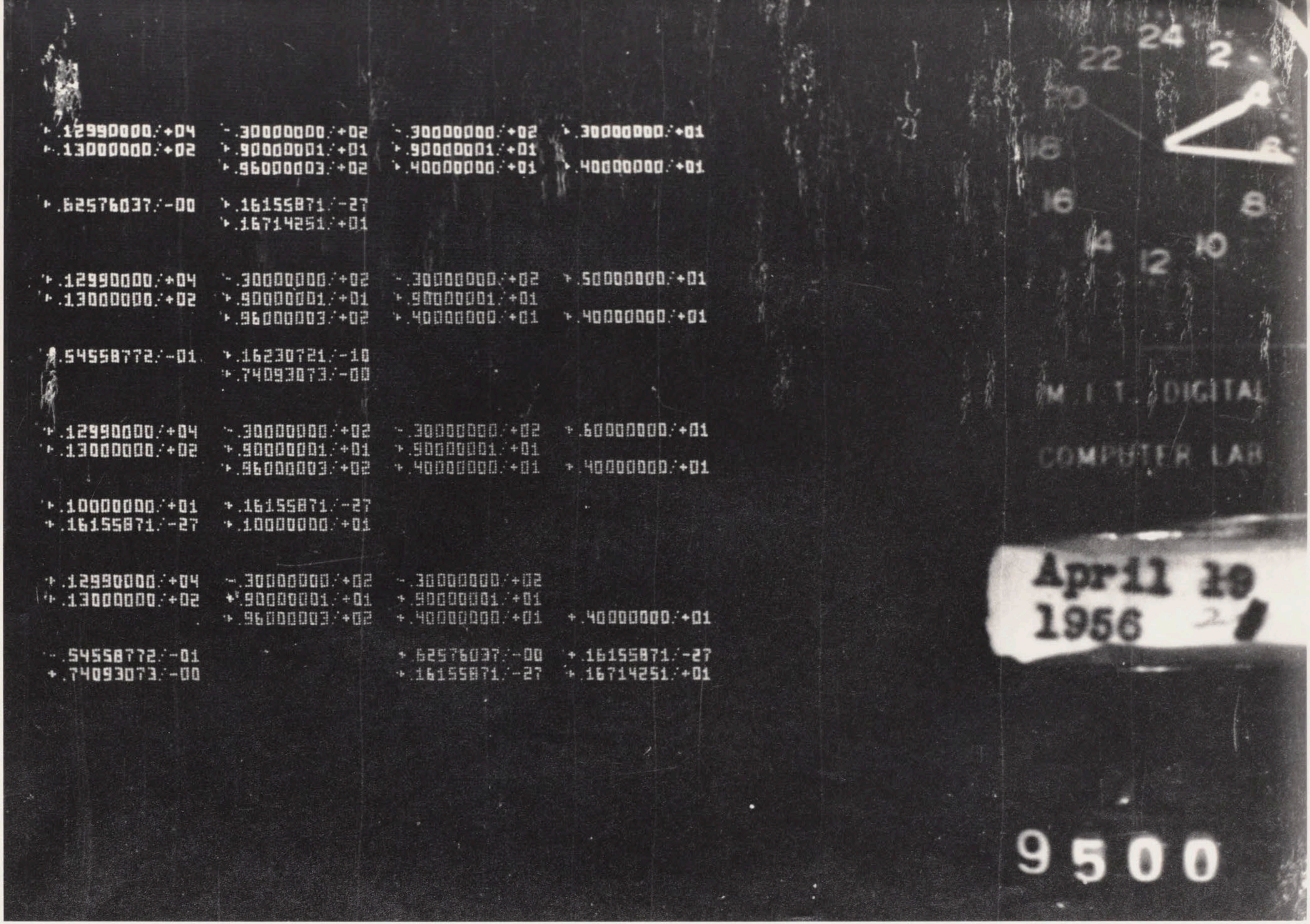

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+.12990000./+04   -.30000000./+02   -.30000000./+02   +.30000000./+01
+.13000000./+02   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.40000000./+01   +.40000000./+01

+.62576037./-00   +.16155871./-27
                  +.16714251./+01


+.12990000./+04   -.30000000./+02   -.30000000./+02   +.50000000./+01
+.13000000./+02   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.40000000./+01   +.40000000./+01

+.54558772./-01   +.16230721./-10
                  +.74093073./-00


+.12990000./+04   -.30000000./+02   -.30000000./+02   +.60000000./+01
+.13000000./+02   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.40000000./+01   +.40000000./+01

+.10000000./+01   +.16155871./-27
+.16155871./-27   +.10000000./+01


+.12990000./+04   -.30000000./+02   -.30000000./+02
+.13000000./+02   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.40000000./+01   +.40000000./+01

-.54558772./-01                     +.62576037./-00   +.16155871./-27
+.74093073./-00                     +.16155871./-27   +.16714251./+01
```

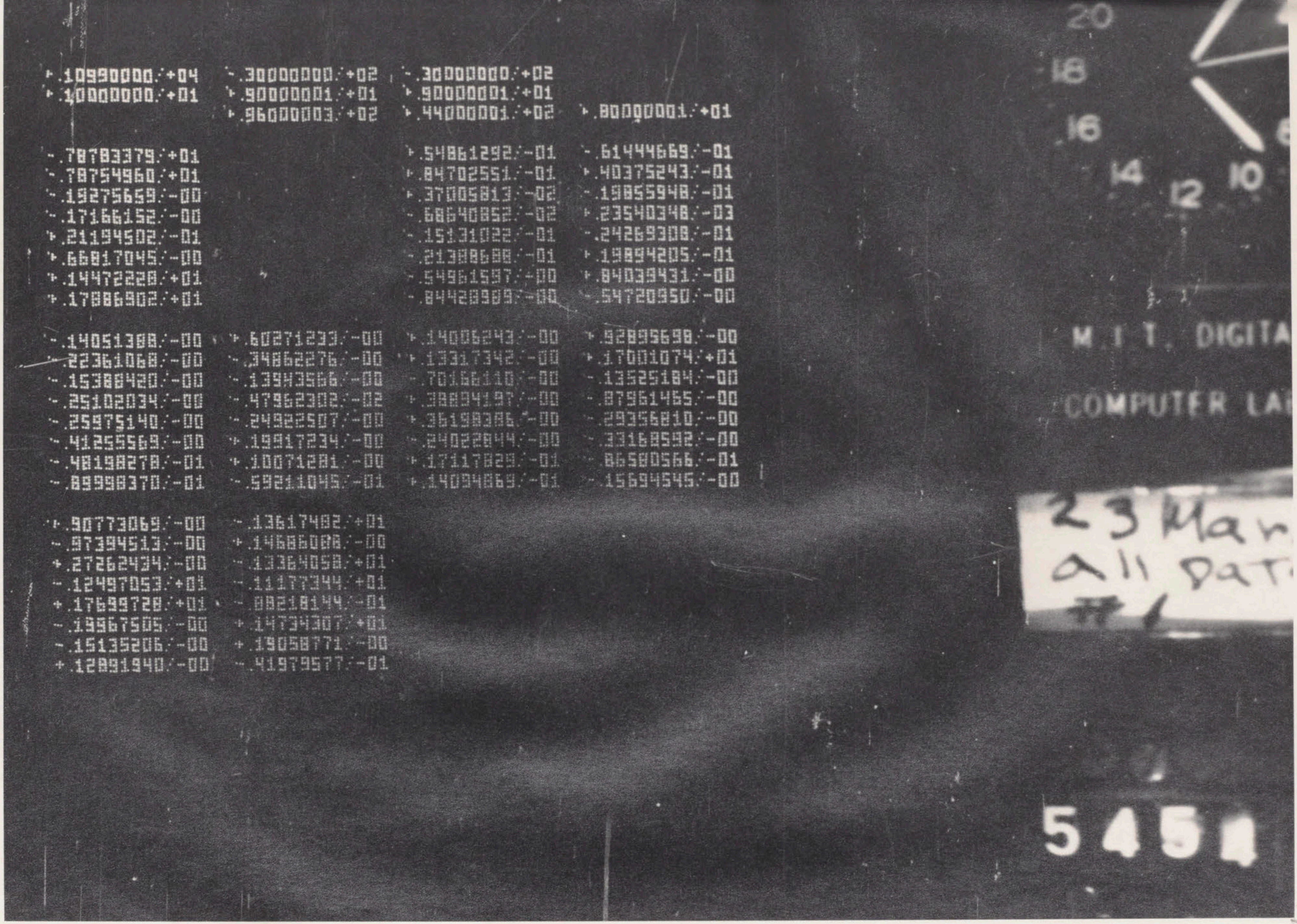
```
+.10990000/+04   -.30000000/+02   -.30000000/+02
+.56843418/-14   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.48000001/+02   +.56843418/-14

-.70783303/+01                    +.50645504/-01   -.61130400/-01
-.19751603/+01                    +.87644323/-01   +.35356666/-01
-.19774156/-00                    -.16845819/-02   -.15059353/-01
-.17423297/-00                    -.29365195/-02   +.86924443/-02
+.35434156/-01                    -.13060878/-01   -.26560742/-01
+.62139880/-00                    -.22668769/-01   +.15323225/-01
+.15120605/+01                    -.50421523/-00   +.86780273/-00
+.17698561/+01                    -.87224543/-00   -.50165331/-00

-.12392529/-00   -.60704970/-00   +.64081721/-01   +.96874660/-00
-.21464890/-00   +.35047972/-00   -.36997590/-01   +.16779186/+01
-.15077243/-00   +.97140438/-01   -.71759748/-00   -.40212801/-00
-.26114526/-00   -.56084953/-01   +.41430515/-00   -.69650560/-00
-.24035869/-00   +.27662834/-00   +.40206477/-00   -.20690850/-00
-.41631221/-00   -.15971273/-00   -.23213225/-00   -.35837617/-00
-.51690366/-01   -.10149083/-00   +.60779312/-02   -.85515930/-01
-.89530936/-01   +.58595485/-01   -.35090970/-02   -.14011795/-00

-.14918413/+01   -.34167909/-00
+.86131572/-00   -.59180021/-00
-.92465472/-00   -.96614880/-00
+.53385275/-00   -.16734174/+01
-.15619248/+01   +.72492808/-00
+.90177565/-00   +.12556178/+01
+.22860729/-00   +.34291151/-01
-.13198654/-00   +.59393253/-01
```

23 Mar.
all Data
#1



```
+.10990000./+04   -.30000000./+02   -.30000000./+02
+.10000000./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.44000001./+02   +.80000001./+01

-.78783379./+01                     +.54861292./-01   -.61444669./-01
-.78754960./+01                     +.84702551./-01   +.40375243./-01
-.19275659./-00                     +.37005813./-02   -.19855948./-01
-.17166152./-00                     -.68640852./-02   +.23540348./-03
+.21194502./-01                     -.15131022./-01   -.24269308./-01
+.66817045./-00                     -.21388688./-01   +.19894205./-01
+.14472228./+01                     -.54961597./-00   +.84039431./-00
+.17886902./+01                     -.84428909./-00   -.54720950./-00

-.14051388./-00   +.60271233./-00   +.14006243./-00   +.92895698./-00
-.22361068./-00   -.34862276./-00   +.13317342./-00   +.17001074./+01
-.15388420./-00   -.13943566./-00   -.70166110./-00   -.13525184./-00
-.25102034./-00   -.47962302./-02   +.38894197./-00   -.87961465./-00
-.25975140./-00   -.24922507./-00   +.36198386./-00   -.29356810./-00
-.41255569./-00   +.19917234./-00   -.24022844./-00   -.33168592./-00
-.48198278./-01   +.10071281./-00   +.17117829./-01   -.86580566./-01
-.89998370./-01   -.59211045./-01   +.14094869./-01   -.15694545./-00

+.90773069./-00   -.13617482./+01
-.97394513./-00   +.14686088./-00
+.27262434./-00   -.13364058./+01
-.12497053./+01   -.11177344./+01
+.17699728./+01   -.88218144./-01
-.19967505./-00   +.14734307./+01
-.15135206./-00   +.19058771./-00
+.12891940./-00   -.41979577./-01
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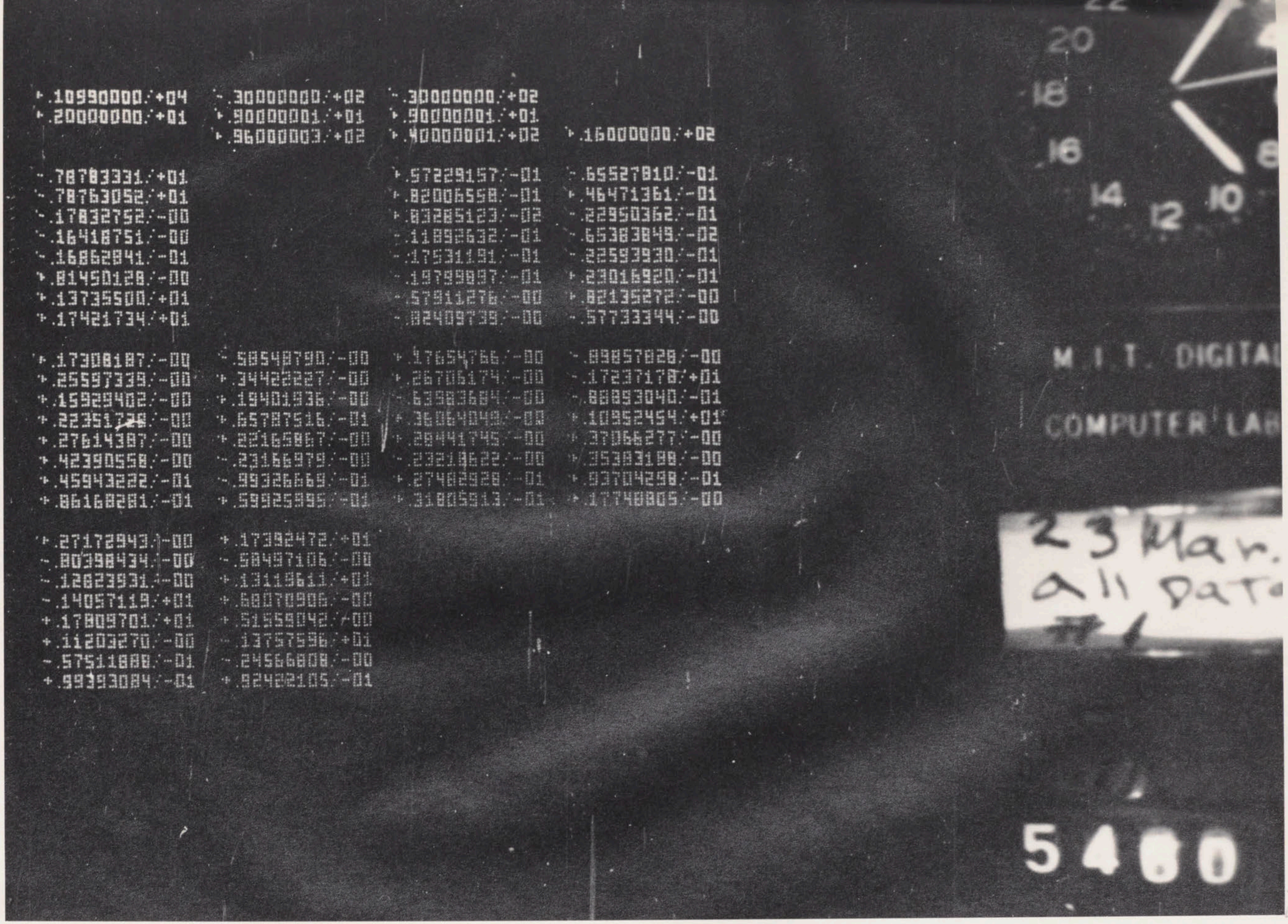
23 Mar
all Data
#1



```
+.10990000:+04   -.30000000:+02   -.30000000:+02
+.20000000:+01   +.90000001:+01   +.90000001:+01
                 +.96000003:+02   +.40000001:+02   +.16000000:+02

-.78783331:+01                    +.57229157:-01   -.65527810:-01
-.78763052:+01                    +.82006558:-01   +.46471361:-01
-.17832752:-00                    +.83285123:-02   -.22950362:-01
-.16418751:-00                    -.11892632:-01   -.65383849:-02
-.16862841:-01                    -.17531191:-01   -.22593930:-01
+.81450128:-00                    -.19799897:-01   +.23016920:-01
+.13735500:+01                    -.57911276:-00   +.82135272:-00
+.17421734:+01                    -.82409739:-00   -.57733344:-00

+.17308187:-00   -.58548790:-00   +.17654766:-00   -.89857828:-00
+.25597339:-00   +.34422227:-00   +.26706174:-00   -.17237178:+01
+.15929402:-00   +.19401936:-00   -.63583684:-00   -.88893040:-01
+.22351728:-00   +.65787516:-01   +.36064049:-00   +.10952454:+01
+.27614387:-00   +.22165867:-00   +.28441745:-00   +.37066277:-00
+.42390558:-00   -.23166979:-00   -.23218622:-00   +.35383188:-00
+.45943222:-01   -.99326669:-01   +.27482920:-01   +.93704298:-01
+.86168281:-01   +.59925995:-01   +.31805513:-01   +.17740805:-00

+.27172943:-00   +.17392472:+01
-.80398434:-00   -.58497106:-00
-.12823931:-00   +.13119611:+01
-.14057119:+01   +.60070906:-00
+.17809701:+01   +.51559042:-00
+.11203270:-00   -.13757596:+01
-.57511888:-01   -.24566808:-00
+.99393084:-01   +.92422105:-01
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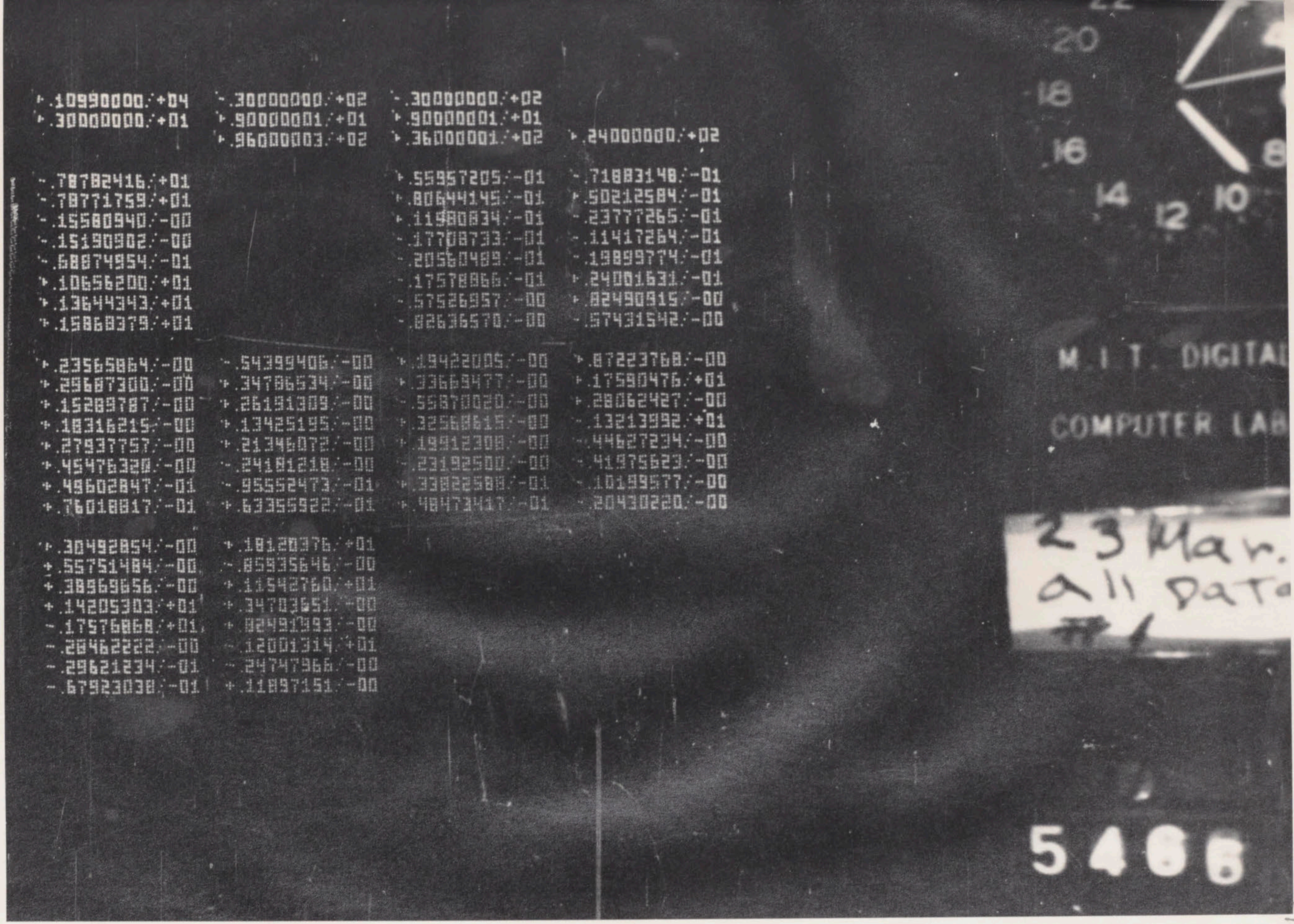


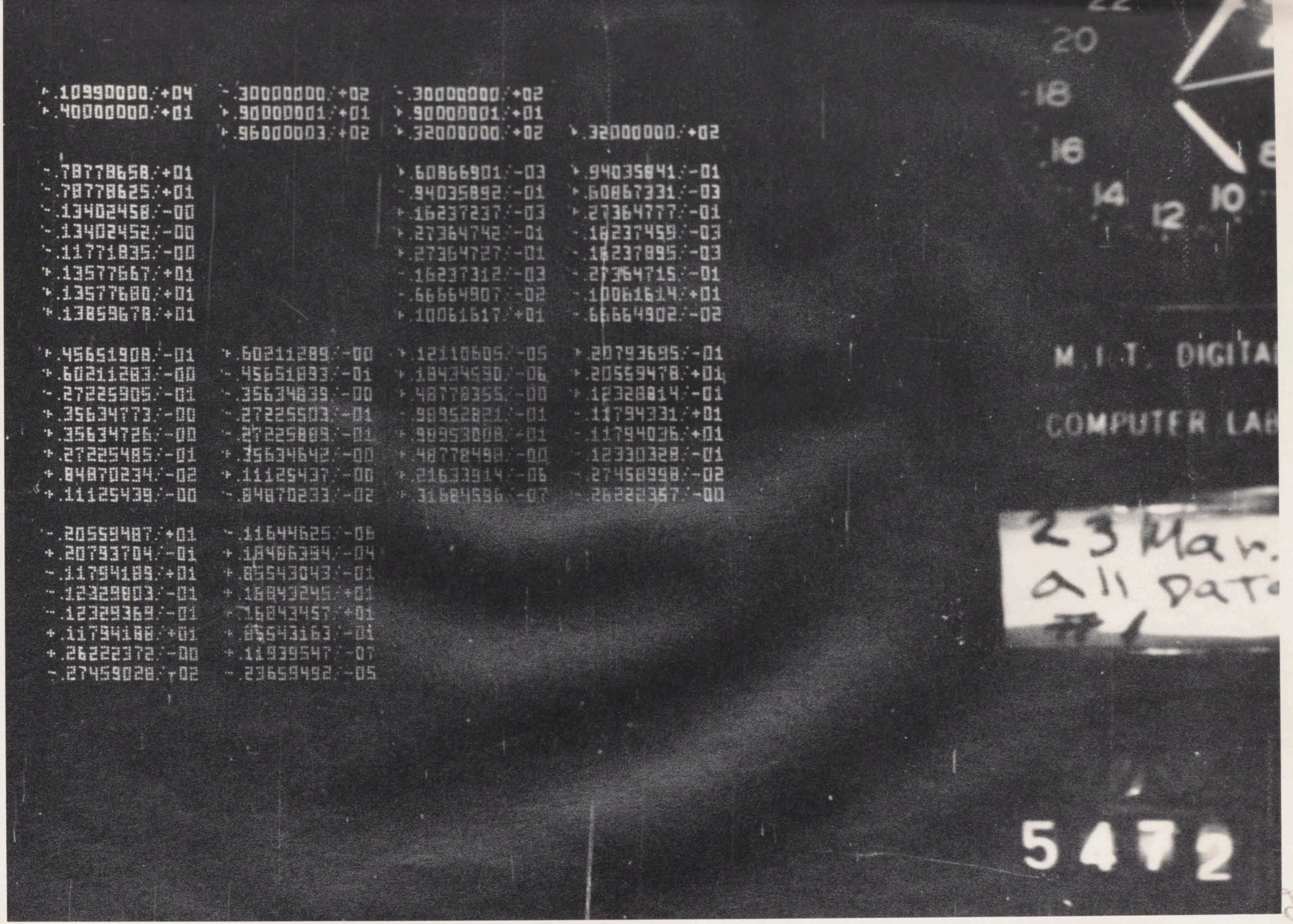
```
+.10990000:+04   -.30000000:+02   -.30000000:+02
+.30000000:+01   +.90000001:+01   +.90000001:+01
                 +.96000003:+02   +.36000001:+02   +.24000000:+02

-.78782416:+01                    +.55957205:-01   -.71883148:-01
-.78771759:+01                    +.80644145:-01   +.50212584:-01
-.15580940:-00                    +.11980834:-01   -.23777265:-01
-.15190902:-00                    -.17708733:-01   -.11417264:-01
-.68874954:-01                    -.20560489:-01   -.19899774:-01
+.10656200:+01                    -.17578866:-01   +.24001631:-01
+.13644343:+01                    -.57526957:-00   +.82490915:-00
+.15868379:+01                    -.82636570:-00   -.57431542:-00

+.23565864:-00   -.54399406:-00   +.19422005:-00   +.87223768:-00
+.29687300:-00   +.34786534:-00   +.33669477:-00   +.17590476:+01
+.15289787:-00   +.26191309:-00   -.55870020:-00   +.28062427:-00
+.18316215:-00   +.13425195:-00   +.32560615:-00   -.13213992:+01
+.27937757:-00   +.21346072:-00   +.19912308:-00   -.44627234:-00
+.45476320:-00   -.24181218:-00   -.23192500:-00   -.41975623:-00
+.49602847:-01   -.95552473:-01   +.33822588:-01   -.10199577:-00
+.76018817:-01   +.63355922:-01   +.48473417:-01   -.20430220:-00

+.30492854:-00   +.18120376:+01
+.55751484:-00   -.85935646:-00
+.38969656:-00   +.11542760:+01
+.14205303:+01   +.34703651:-00
-.17576868:+01   +.82491393:-00
-.28462222:-00   -.12001314:+01
-.29621234:-01   -.24747966:-00
-.67923038:-01   +.11897151:-00
```

23 Mar.
all Data
#1



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+.40000000.:+01   +.90000001.:+01   +.90000001.:+01
                  +.96000003.:+02   +.32000000.:+02   +.32000000.:+02

-.78778658.:+01                     +.60866901.:-03   +.94035841.:-01
-.78778625.:+01                     -.94035892.:-01   +.60867331.:-03
-.13402458.:-00                     +.16237237.:-03   +.27364777.:-01
-.13402452.:-00                     +.27364742.:-01   -.16237459.:-03
-.11771835.:-00                     +.27364727.:-01   -.16237895.:-03
+.13577667.:+01                     -.16237312.:-03   -.27364715.:-01
+.13577680.:+01                     -.66664907.:-02   -.10061614.:+01
+.13859678.:+01                     +.10061617.:+01   -.66664902.:-02

+.45651908.:-01   +.60211289.:-00   +.12110605.:-05   +.20793695.:-01
+.60211283.:-00   -.45651893.:-01   +.18434590.:-06   +.20559478.:+01
-.27225905.:-01   -.35634839.:-00   +.48778355.:-00   +.12328814.:-01
+.35634773.:-00   -.27225503.:-01   -.98952821.:-01   -.11794331.:+01
+.35634726.:-00   -.27225809.:-01   +.98953008.:-01   -.11794036.:+01
+.27225485.:-01   +.35634642.:-00   +.48778498.:-00   -.12330328.:-01
+.84870234.:-02   +.11125437.:-00   +.21633914.:-06   -.27458998.:-02
+.11125439.:-00   -.84870233.:-02   +.31684596.:-07   -.26222367.:-00

-.20559487.:+01   -.11644625.:-06
+.20793704.:-01   +.18486394.:-04
-.11794189.:+01   +.85543043.:-01
-.12329803.:-01   +.16843245.:+01
-.12329369.:-01   -.16843457.:+01
+.11794188.:+01   +.85543163.:-01
+.26222372.:-00   +.11939547.:-07
-.27459028.:+02   -.23659492.:-05
```

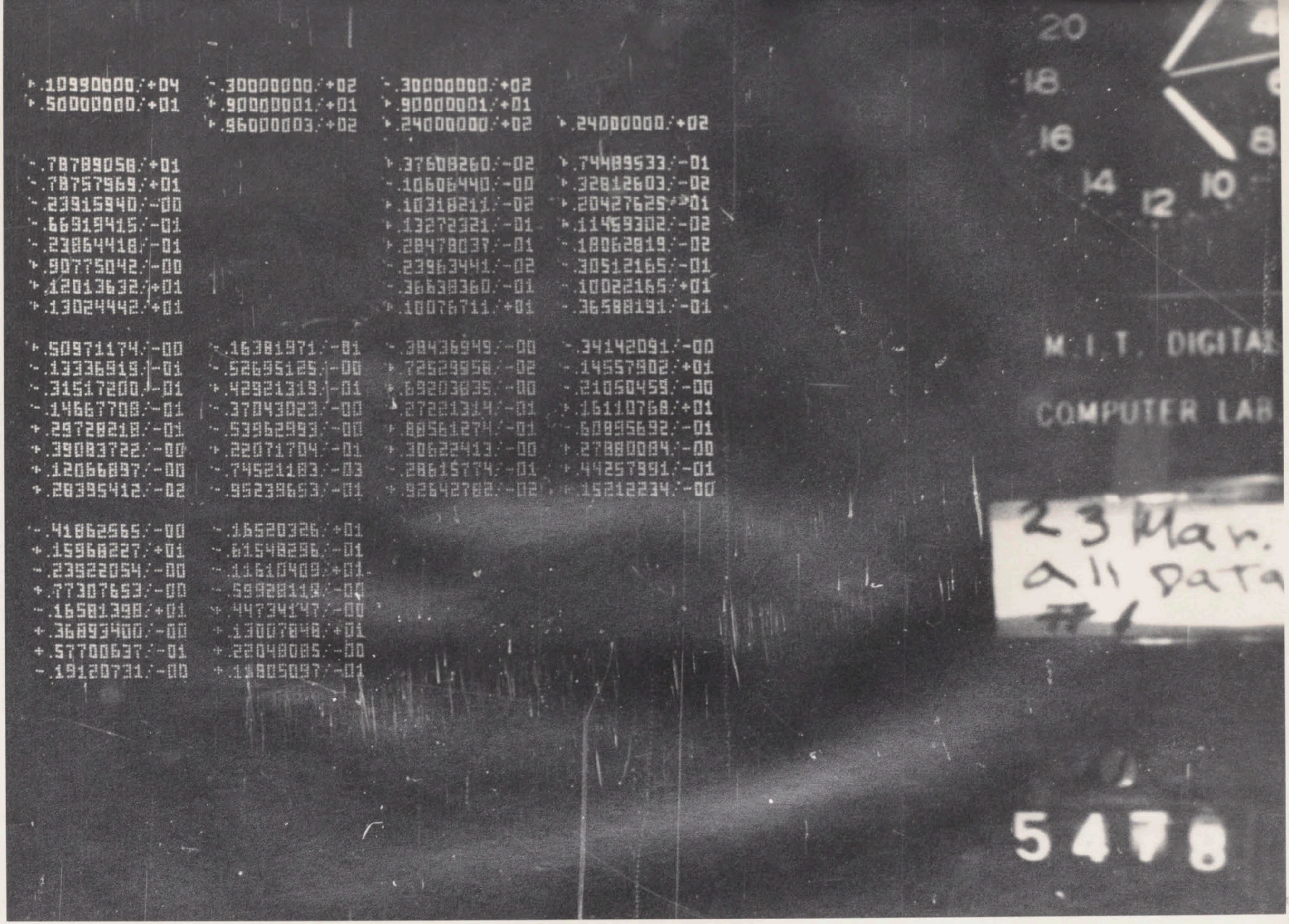

```
+.10990000.:+04   -.30000000.:+02   -.30000000.:+02
+.50000000.:+01   +.90000001.:+01   +.90000001.:+01
                  +.96000003.:+02   +.24000000.:+02   +.24000000.:+02

-.78789058.:+01                     +.37608260.:-02   +.74489533.:-01
-.78757969.:+01                     -.10606440.:-00   +.32812603.:-02
-.23915940.:-00                     +.10318211.:-02   +.20427625.:[illegible]01
-.66919415.:-01                     +.13272321.:-01   +.11469302.:-02
-.23864418.:-01                     +.28478037.:-01   -.18062819.:-02
+.90775042.:-00                     -.23963441.:-02   -.30512165.:-01
+.12013632.:+01                     -.36638360.:-01   -.10022165.:+01
+.13024442.:+01                     +.10076711.:+01   -.36588191.:-01

+.50971174.:-00   -.16381971.:-01   -.38436949.:-00   -.34142091.:-00
-.13336919.:-01   -.52695125.:-00   +.72529958.:-02   -.14557902.:+01
-.31517200.:-01   +.42921319.:-01   +.69203835.:-00   -.21050459.:-00
-.14667708.:-01   -.37043023.:-00   +.27221314.:-01   +.16110768.:+01
+.29728218.:-01   -.53962993.:-00   +.80561274.:-01   -.60895692.:-01
+.39083722.:-00   +.22071704.:-01   +.30622413.:-00   +.27880084.:-00
+.12066897.:-00   -.74521183.:-03   -.28615774.:-01   +.44257991.:-01
+.28395412.:-02   -.95239653.:-01   +.92642782.:-02   +.15212234.:-00

-.41862565.:-00   -.16520326.:+01
+.15968227.:+01   -.61548296.:-01
-.23922054.:-00   -.11610409.:+01
+.77307653.:-00   -.59928118.:-00
-.16581398.:+01   +.44734147.:-00
+.36893400.:-00   +.13007848.:+01
+.57700637.:-01   +.22048085.:-00
-.19120731.:-00   +.11805097.:-01
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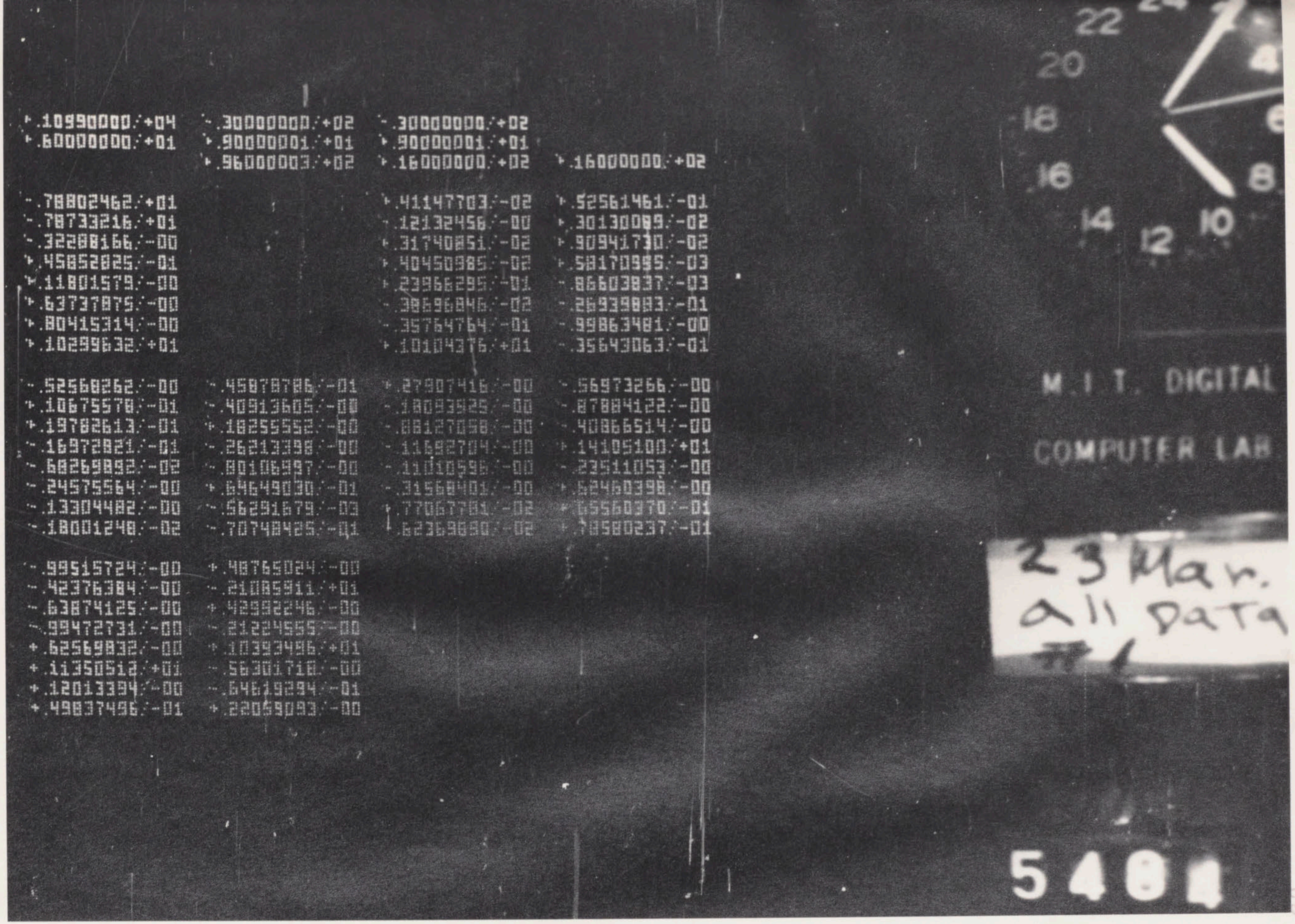

```
+.10990000:+04  -.30000000:+02  -.30000000:+02
+.60000000:+01  +.90000001:+01  +.90000001:+01
                +.96000003:+02  +.16000000:+02  +.16000000:+02

-.78802462:+01                  +.41147703:-02  +.52561461:-01
-.78733216:+01                  -.12132456:-00  +.30130089:-02
-.32208166:-00                  +.31740851:-02  +.90941730:-02
+.45852025:-01                  +.40450985:-02  +.58170995:-03
+.11801579:-00                  +.23966295:-01  -.86603837:-03
+.63737875:-00                  -.38696846:-02  -.26939883:-01
+.80415314:-00                  -.35764764:-01  -.99863481:-00
+.10299632:+01                  +.10104376:+01  -.35643063:-01

-.52560262:-00  -.45878786:-01  +.27907416:-00  -.56973266:-00
+.10675570:-01  -.40913605:-00  -.18093925:-00  -.87804122:-00
+.19782613:-01  +.18255552:-00  -.08127058:-00  -.40866514:-00
-.16972821:-01  -.26213398:-00  -.11692704:-00  +.14105100:+01
-.60269892:-02  -.80106997:-00  -.11010596:-00  -.23511053:-00
-.24575564:-00  +.64649030:-01  -.31560401:-00  +.62460398:-00
-.13304482:-00  -.56291679:-03  +.77067781:-02  +.65560370:-01
-.18001240:-02  -.70748425:-01  +.62369890:-02  +.78580237:-01

-.99515724:-00  +.48765024:-00
-.42376384:-00  -.21085911:+01
-.63874125:-00  +.42992246:-00
-.99472731:-00  -.21224555:-00
+.62569832:-00  +.10393496:+01
+.11350512:+01  -.56301718:-00
+.12013394:-00  -.64619294:-01
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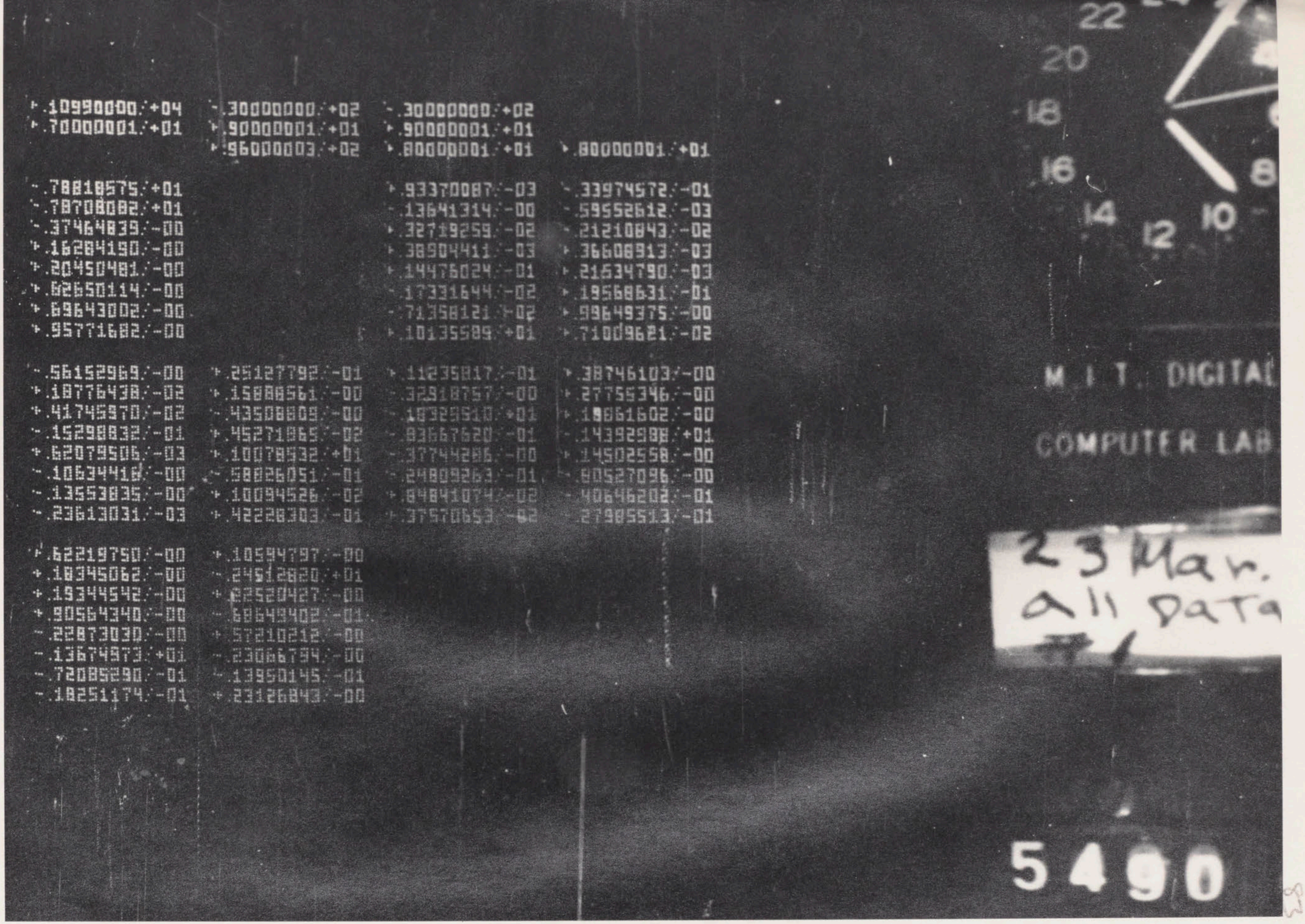
M.I.T. DIGITAL

COMPUTER LAB

23 Mar.
all Data
#1

5484



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+.10990000:+04   -.30000000:+02   -.30000000:+02
+.70000001:+01   +.90000001:+01   +.90000001:+01
                 +.96000003:+02   +.80000001:+01   +.80000001:+01

-.78810575:+01                    +.93370087:-03   -.33974572:-01
-.78708082:+01                    -.13641314:-00   -.59552612:-03
-.37464839:-00                    +.32719259:-02   -.21210843:-02
+.16284190:-00                    +.38904411:-03   +.36608913:-03
+.20450481:-00                    +.14476024:-01   +.21634790:-03
+.62650114:-00                    -.17331644:-02   +.19568631:-01
+.69643002:-00                    -.71358121:+02   +.99649375:-00
+.95771682:-00                    +.10135589:+01   +.71009621:-02

-.56152969:-00   +.25127792:-01   +.11235817:-01   +.38746103:-00
+.18776438:-02   +.15888561:-00   -.32918757:-00   +.27755346:-00
+.41745970:-02   -.43508809:-00   -.10329510:+01   +.19861602:-00
-.15298832:-01   +.45271865:-02   -.83667620:-01   -.14392988:+01
+.62079506:-03   +.10078932:+01   -.37744206:-00   +.14502558:-00
-.10634416:-00   -.58026051:-01   -.24809263:-01   -.80527096:-00
-.13553835:-00   +.10094526:-02   +.84841074:-02   -.40646202:-01
-.23613031:-03   +.42228303:-01   +.37570653:-02   -.27985513:-01

+.62219750:-00   +.10594797:-00
+.18345062:-00   -.24512820:+01
+.19344542:-00   +.22520427:-00
+.90564340:-00   -.68649402:-01
-.22873030:-00   +.57210212:-00
-.13674973:+01   -.23066794:-00
-.72085290:-01   -.13950145:-01
-.18251174:-01   +.23126843:-00
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23 Mar.
all Data
#1

5490

```
+.10990000./+04   -.30000000./+02   -.30000000./+02
+.80000001./+01   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.56843418./-14   +.56843418./-14

-.78692957./+01                     +.23658292./-01   +.16155871./-27
-.78825122./+01                     +.16155871./-27   -.14202126./-00
-.39361965./-00                     +.79593432./-09   +.16155871./-27
+.68007785./-00                     +.16155871./-27   -.14188863./-08
+.21488982./-00                     -.77100791./-09   +.16155871./-27
+.68007802./-00                     +.16155871./-27   +.13370918./-08
+.21488983./-00                     -.99507653./-00   +.16155871./-27
+.93541061./-00                     +.16155871./-27   +.10144879./+01

-.57110351./-00   +.16155871./-27   -.14158546./-08   +.16155871./-27
+.16155871./-27   +.59426852./-07   +.16155871./-27   -.21639604./-06
+.39897840./-08   +.16155871./-27   +.17279767./-00   +.16155871./-27
+.16155871./-27   +.23840671./-00   +.16155871./-27   +.16817648./+01
-.35316787./-08   +.16155871./-27   +.11447709./+01   +.16155871./-27
+.16155871./-27   -.16817647./+01   +.16155871./-27   +.23840679./-00
-.13629339./-00   +.16155871./-27   -.89482796./-09   +.16155871./-27
+.16155871./-27   -.44554355./-08   +.16155871./-27   +.20212278./-07

+.21876167./-08   +.16155871./-27
+.16155871./-27   -.25428281./+01
+.11447709./+01   +.16155871./-27
+.16155871./-27   -.13746819./-06
-.17273770./-00   +.16155871./-27
+.16155871./-27   -.59666703./-07
+.13018006./-08   +.16155871./-27
+.16155871./-27   +.22907587./-00
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23 Mar.
all Data
#1

5496

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+.90000001/+01   +.90000001/+01   +.90000001/+01
                 +.96000003/+02   +.12000000/+02   +.56843418/-14

-.78820172/+01                    +.12857950/-03   +.31681634/-01
-.78704792/+01                    +.13782602/-00   +.32006058/-03
-.37926483/-00                    -.89759900/-02   +.92565261/-03
+.17361319/-00                    -.11289440/-02   -.91113791/-02
+.20905998/-00                    -.95605234/-02   +.12360902/-02
+.63712209/-00                    +.49691973/-03   -.15030212/-01
+.69634342/-00                    -.12884600/-02   -.99619537/-00
+.95301109/-00                    -.10138120/+01   +.11921662/-02

-.56438821/-00   +.17669611/-02   +.27061572/-01   +.38556614/-00
+.22187798/-02   +.12029429/-00   -.30868142/-00   +.60601344/-01
+.23027253/-03   +.86209140/-01   -.11058583/+01   -.20656296/-01
-.56867357/-01   +.40887959/-01   -.39537470/-01   -.16546724/+01
+.24302599/-02   +.11116823/+01   +.13799206/-00   +.22707743/-00
-.71095949/-01   -.28709694/-01   -.58253556/-01   -.11485616/-00
-.13568536/-00   -.73597160/-02   +.86302722/-04   -.40960978/-01
-.33377282/-03   +.37662941/-01   +.31316271/-02   +.67252377/-02

+.52317410/-00   +.46167802/-01
+.29332703/-00   -.24717877/+01
+.19492305/-00   +.42667260/-00
+.19590283/-00   +.96796639/-01
+.13928525/-01   +.34221348/-00
-.16434647/+01   -.19562336/-00
-.61065226/-01   -.77240144/-02
-.28712067/-01   +.23075586/-00
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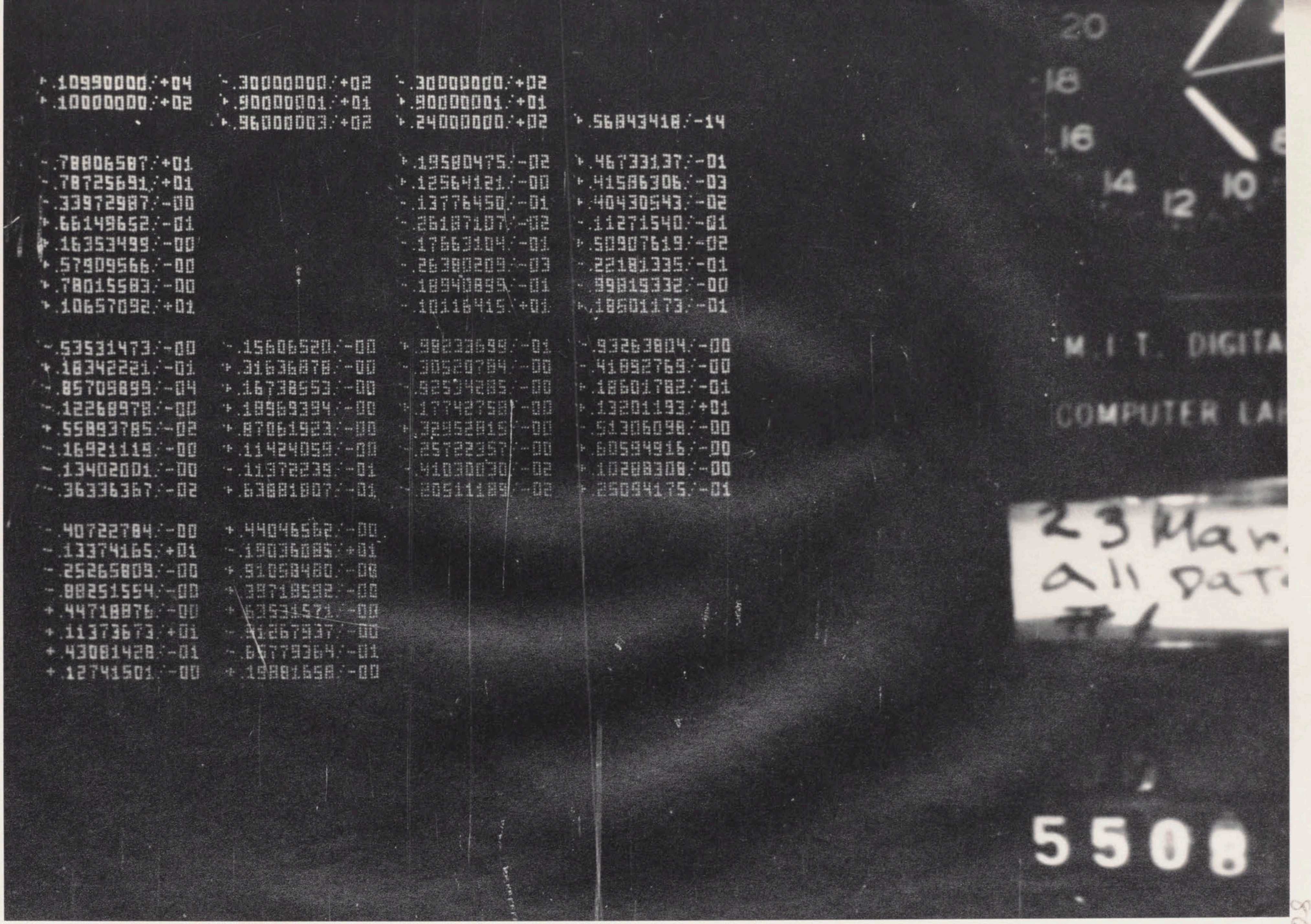

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+.10990000.:+04   -.30000000.:+02   -.30000000.:+02
+.10000000.:+02   +.90000001.:+01   +.90000001.:+01
                  +.96000003.:+02   +.24000000.:+02   +.56843418.:-14

-.78806587.:+01                     +.19580475.:-02   +.46733137.:-01
-.78725691.:+01                     +.12564121.:-00   +.41586306.:-03
-.33972987.:-00                     -.13776450.:-01   +.40430543.:-02
+.66149652.:-01                     -.26187107.:-02   -.11271540.:-01
+.16353499.:-00                     -.17663104.:-01   +.50907619.:-02
+.57909566.:-00                     -.26380209.:-03   -.22181335.:-01
+.78015583.:-00                     -.18940899.:-01   -.99819332.:-00
+.10657092.:+01                     -.10116415.:+01   +.18601173.:-01

-.53531473.:-00   -.15606520.:-00   +.98233699.:-01   -.93263804.:-00
+.18342221.:-01   +.31636878.:-00   -.30520784.:-00   -.41892769.:-00
-.85709899.:-04   +.16738553.:-00   -.92534285.:-00   +.18601782.:-01
-.12268978.:-00   +.18969394.:-00   +.17742758.:-00   +.13201193.:+01
+.55893785.:-02   +.87061923.:-00   +.32952815.:-00   -.51306098.:-00
-.16921119.:-00   +.11424059.:-00   -.25722357.:-00   +.60594916.:-00
-.13402001.:-00   -.11372239.:-01   +.41030030.:-02   +.10288308.:-00
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-.40722784.:-00   +.44046562.:-00
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-.25265809.:-00   +.91058480.:-00
-.88251554.:-00   +.39718592.:-00
+.44718876.:-00   +.63531571.:-00
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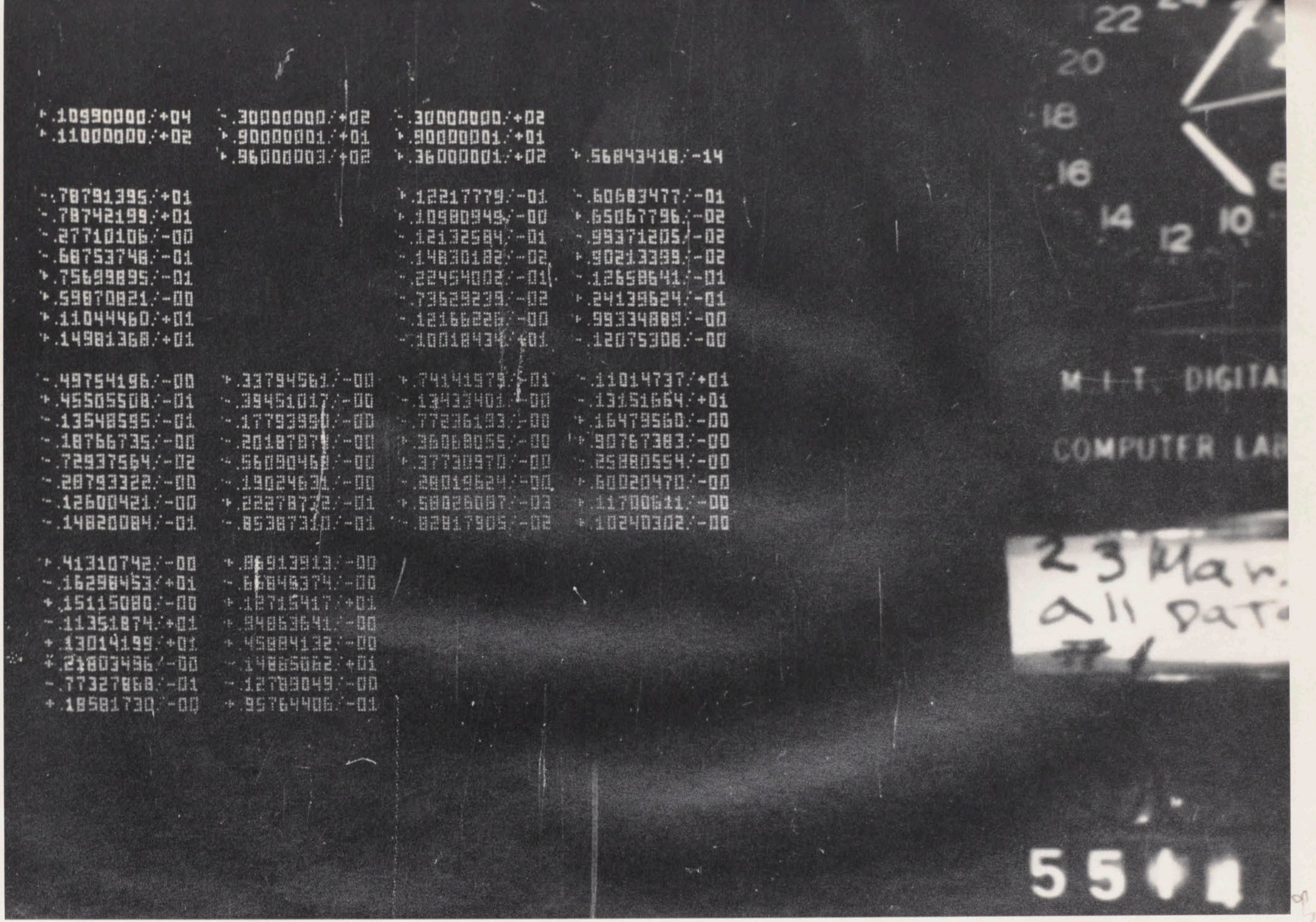

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+.10990000./+04   -.30000000./+02   -.30000000./+02
+.11000000./+02   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.36000001./+02   +.56843418./-14

-.78791395./+01                     +.12217779./-01   -.60683477./-01
-.78742199./+01                     +.10980949./-00   +.65067796./-02
-.27710106./-00                     -.12132584./-01   -.99371205./-02
-.68753748./-01                     -.14830182./-02   +.90213399./-02
+.75699895./-01                     -.22454002./-01   -.12658641./-01
+.59870821./-00                     -.73629239./-02   +.24139624./-01
+.11044460./+01                     -.12166226./-00   +.99334889./-00
+.14981368./+01                     -.10018434./+01   -.12075308./-00

-.49754196./-00   +.33794561./-00   +.74141979./-01   -.11014737./+01
+.45505508./-01   -.39451017./-00   -.13433401./-00   -.13151664./+01
-.13548595./-01   -.17793990./-00   -.77236193./-00   +.16479560./-00
-.18766735./-00   -.20187879./-00   +.36068055./-00   +.90767383./-00
-.72937564./-02   -.56090468./-00   +.37730970./-00   -.25880554./-00
-.28793322./-00   -.19024631./-00   -.28019624./-00   +.60020470./-00
-.12600421./-00   +.22278772./-01   +.58026087./-03   +.11700611./-00
-.14820084./-01   -.85387310./-01   -.82817905./-02   +.10240302./-00

+.41310742./-00   +.86913913./-00
-.16298453./+01   -.66846374./-00
+.15115080./-00   +.12715417./+01
-.11351874./+01   +.94863641./-00
+.13014199./+01   +.45884132./-00
+.21803496./-00   -.14865062./+01
-.77327868./-01   -.12783049./-00
+.18581730./-00   +.95764406./-01
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+.12990000./+04   -.30000000./+02   -.30000000./+02
+.56043418./-14   +.90000001./+01   +.90000001./+01
                  +.96000003./+02   +.40000001./+02   +.40000000./+01

-.78785391./+01                     +.27148567./-01   -.66481127./-01
-.78750554./+01                     +.10011155./-00   +.18614415./-01
-.23481604./-00                     -.58480175./-02   -.16327336./-01
-.12891915./-00                     -.28734614./-02   +.48378873./-02
+.43040826./-01                     -.22217588./-01   -.17940057./-01
+.61205673./-00                     -.13360296./-01   +.25066776./-01
+.13201420./+01                     -.27367451./-00   +.96433985./-00
+.17809524./+01                     -.97010671./-00   -.27232924./-00

-.47938510./-00   -.38233047./-00   -.12130687./-00   -.10154546./+01
+.43032746./-01   +.40648403./-00   +.31730611./-02   -.15563966./+01
-.27925902./-01   +.18451614./-00   +.73565620./-00   +.15479432./-00
-.19602677./-00   +.18444406./-00   -.37708470./-00   +.88538634./-00
-.38570061./-01   +.44835612./-00   -.37636074./-00   +.10805428./-01
-.36910310./-00   +.14564661./-00   +.26751783./-00   +.44461822./-00
-.11488564./-00   -.37204380./-01   -.83427838./-02   +.10105907./-00
-.26406271./-01   +.95329336./-01   -.16179534./-02   +.13098843./-00

+.69943189./-00   +.11523385./+01
-.13667621./+01   -.29531553./-00
+.25922778./-00   +.13424657./+01
-.11812133./+01   +.11015352./+01
+.16103039./+01   +.24377264./-00
-.70717363./-01   -.15516629./+01
-.12336896./-00   -.16615413./-00
+.16954392./-00   +.58740451./-01
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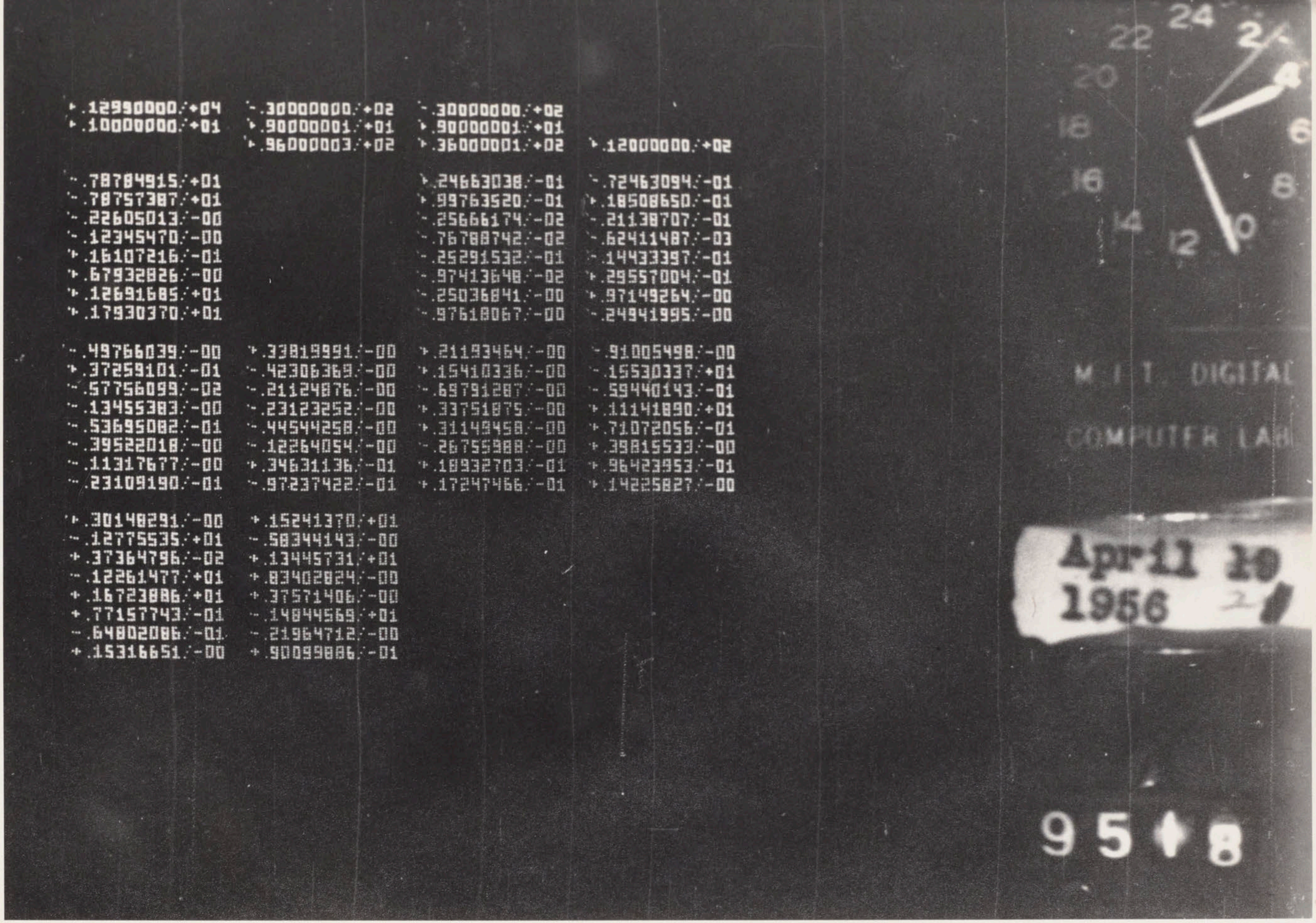

```
+.12990000./+04  -.30000000./+02  -.30000000./+02
+.10000000./+01  +.90000001./+01  +.90000001./+01
                 +.96000003./+02  +.36000001./+02  +.12000000./+02

-.78784915./+01                   +.24663038./-01  -.72463094./-01
-.78757387./+01                   +.99763520./-01  +.18508650./-01
-.22605013./-00                   -.25666174./-02  -.21138707./-01
-.12345470./-00                   -.76788742./-02  -.62411487./-03
+.16107216./-01                   -.25291532./-01  -.14433397./-01
+.67932826./-00                   -.97413648./-02  +.29557004./-01
+.12691685./+01                   -.25036841./-00  +.97149264./-00
+.17930370./+01                   -.97618067./-00  -.24941995./-00

-.49766039./-00  +.33819991./-00  +.21193464./-00  -.91005498./-00
+.37259101./-01  -.42306369./-00  +.15410336./-00  -.15530337./+01
-.57756099./-02  -.21124876./-00  -.69791287./-00  -.59440143./-01
-.13455383./-00  -.23123252./-00  +.33751875./-00  +.11141890./+01
-.53695082./-01  -.44544258./-00  +.31149458./-00  +.71072056./-01
-.39522018./-00  -.12264054./-00  -.26755988./-00  +.39815533./-00
-.11317677./-00  +.34631136./-01  +.18932703./-01  +.96423953./-01
-.23109190./-01  -.97237422./-01  +.17247466./-01  +.14225827./-00

+.30148291./-00  +.15241370./+01
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+.37364796./-02  +.13445731./+01
-.12261477./+01  +.83402824./-00
+.16723886./+01  +.37571406./-00
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-.64802086./-01  -.21964712./-00
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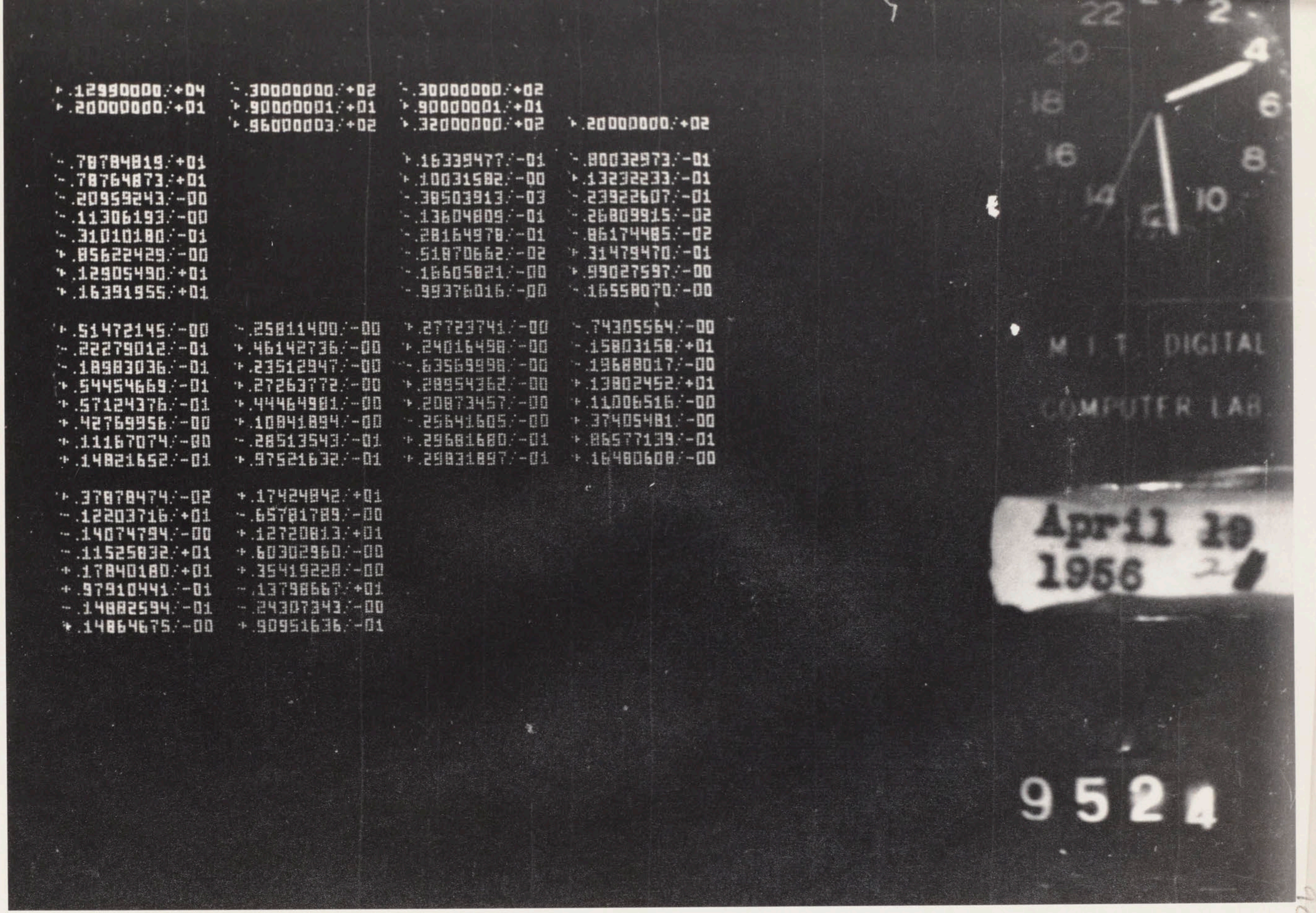

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-.78784819./+01                     +.16339477./-01   -.80032973./-01
-.78764873./+01                     +.10031582./-00   +.13232233./-01
-.20959243./-00                     -.38503913./-03   -.23922607./-01
-.11306193./-00                     -.13604809./-01   -.26809915./-02
-.31010180./-01                     -.28164978./-01   -.86174485./-02
+.85622429./-00                     -.51870662./-02   +.31479470./-01
+.12905490./+01                     -.16605821./-00   +.99027597./-00
+.16391955./+01                     -.99376016./-00   -.16558070./-00

+.51472145./-00   -.25811400./-00   +.27723741./-00   -.74305564./-00
-.22279012./-01   +.46142736./-00   +.24016498./-00   -.15803158./+01
-.18983036./-01   +.23512947./-00   -.63569998./-00   -.19688017./-00
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+.57124376./-01   +.44464901./-00   +.20873457./-00   +.11006516./-00
+.42769956./-00   +.10841894./-00   -.25641605./-00   +.37405481./-00
+.11167074./-00   -.28513543./-01   +.29681680./-01   +.86577139./-01
+.14821652./-01   +.97521632./-01   +.29831897./-01   +.16480608./-00

+.37878474./-02   +.17424842./+01
-.12203716./+01   -.65781789./-00
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-.11525832./+01   +.60302960./-00
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-.14882594./-01   -.24307343./-00
+.14864675./-00   +.90951636./-01
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+.30000000:+01   +.90000001:+01   +.90000001:+01
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-.78790351:+01                    +.32483406:-02   -.69872482:-01
-.78752814:+01                    +.10833171:-00   +.13626726:-02
-.25981438:-00                    -.50891023:-02   -.18268376:-01
-.63755868:-01                    -.85589698:-02   -.11143828:-03
+.23016795:-01                    -.27993602:-01   -.44651925:-02
+.69229882:-00                    +.13020643:-03   +.30893756:-01
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+.31633630:-01   -.56534856:-00   -.20760932:-00   -.13513915:-00
+.35141527:-00   -.10508432:-00   +.31043037:-00   +.42860791:-00
+.12311168:-00   +.15871342:-01   -.18410487:-01   +.86800090:-01
+.10831746:-01   -.91777651:-01   -.12379641:-01   +.12080115:-00

-.16980248:-00   +.14624086:+01
-.15044552:+01   -.88611441:-00
-.19686029:-00   +.11881091:+01
-.10458716:+01   +.57594031:-00
+.15249791:+01   +.45253092:-00
+.28062295:-00   -.13709756:+01
+.79786032:-02   -.20496153:-00
+.17199552:-00   +.11177031:-00
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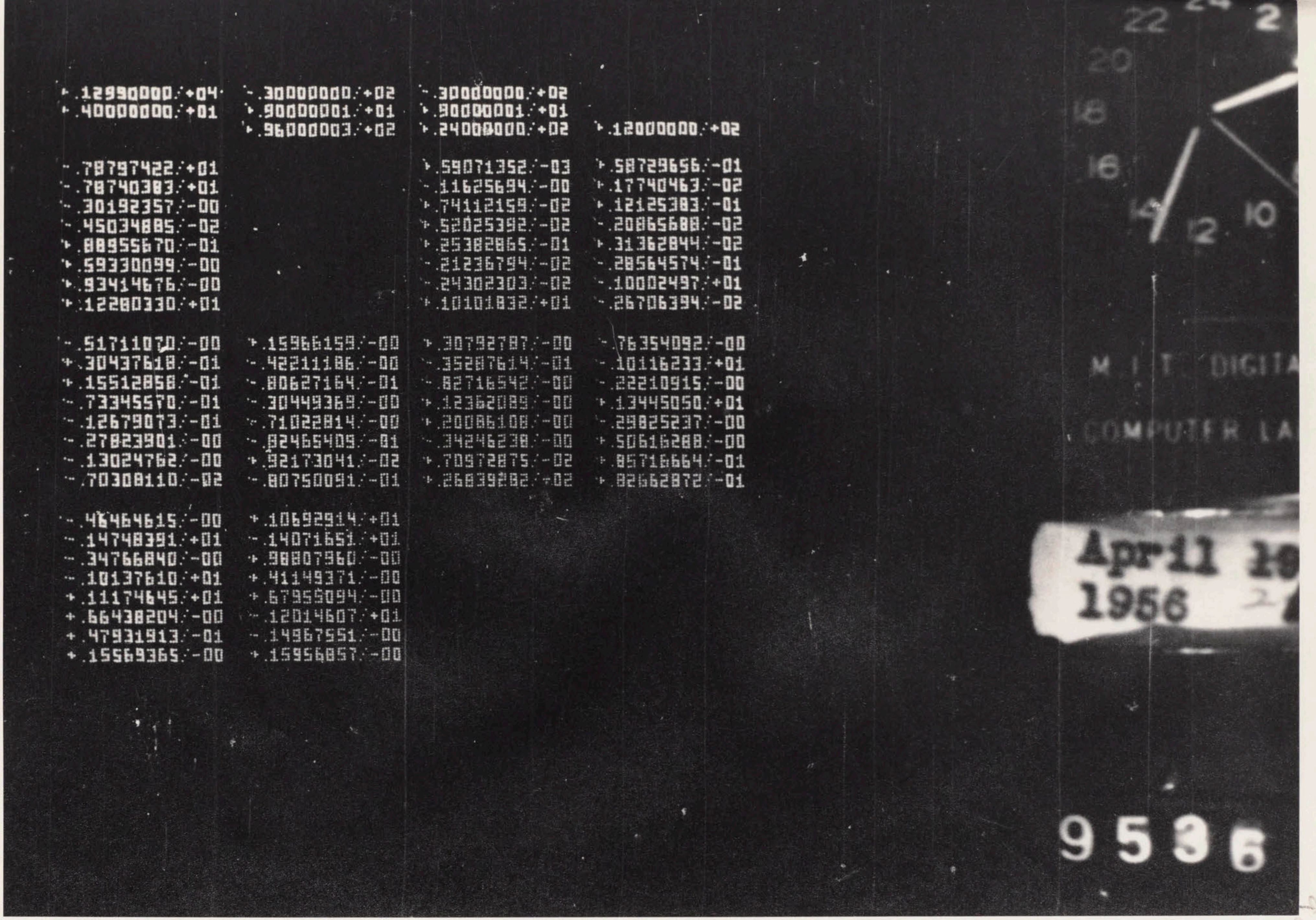

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+.40000000:+01  +.90000001:+01  +.90000001:+01
                +.96000003:+02  +.24000000:+02  +.12000000:+02

-.78797422:+01                  +.59071352:-03  +.58729656:-01
-.78740383:+01                  -.11625694:-00  +.17740463:-02
-.30192357:-00                  +.74112159:-02  +.12125383:-01
-.45034885:-02                  +.52025392:-02  -.20865688:-02
+.88955670:-01                  +.25382865:-01  +.31362844:-02
+.59330099:-00                  -.21236794:-02  -.28564574:-01
+.93414676:-00                  -.24302303:-02  -.10002497:+01
+.12280330:+01                  +.10101832:+01  -.26706394:-02

-.51711070:-00  +.15966159:-00  +.30792787:-00  -.76354092:-00
+.30437618:-01  -.42211186:-00  -.35287614:-01  -.10116233:+01
+.15512858:-01  -.80627164:-01  -.82716542:-00  -.22210915:-00
-.73345570:-01  -.30449369:-00  +.12362089:-00  +.13445050:+01
-.12679073:-01  -.71022814:-00  +.20086108:-00  -.29825237:-00
-.27823901:-00  -.82465409:-01  -.34246238:-00  +.50616288:-00
-.13024762:-00  +.92173041:-02  +.70972875:-02  +.85716664:-01
-.70308110:-02  -.80750091:-01  +.26839282:+02  +.82662872:-01

-.46464615:-00  +.10692914:+01
-.14748391:+01  -.14071651:+01
-.34766840:-00  +.98807960:-00
-.10137610:+01  +.41149371:-00
+.11174645:+01  +.67955094:-00
+.66438204:-00  -.12014607:+01
+.47931913:-01  -.14967551:-00
+.15569365:-00  +.15956857:-00
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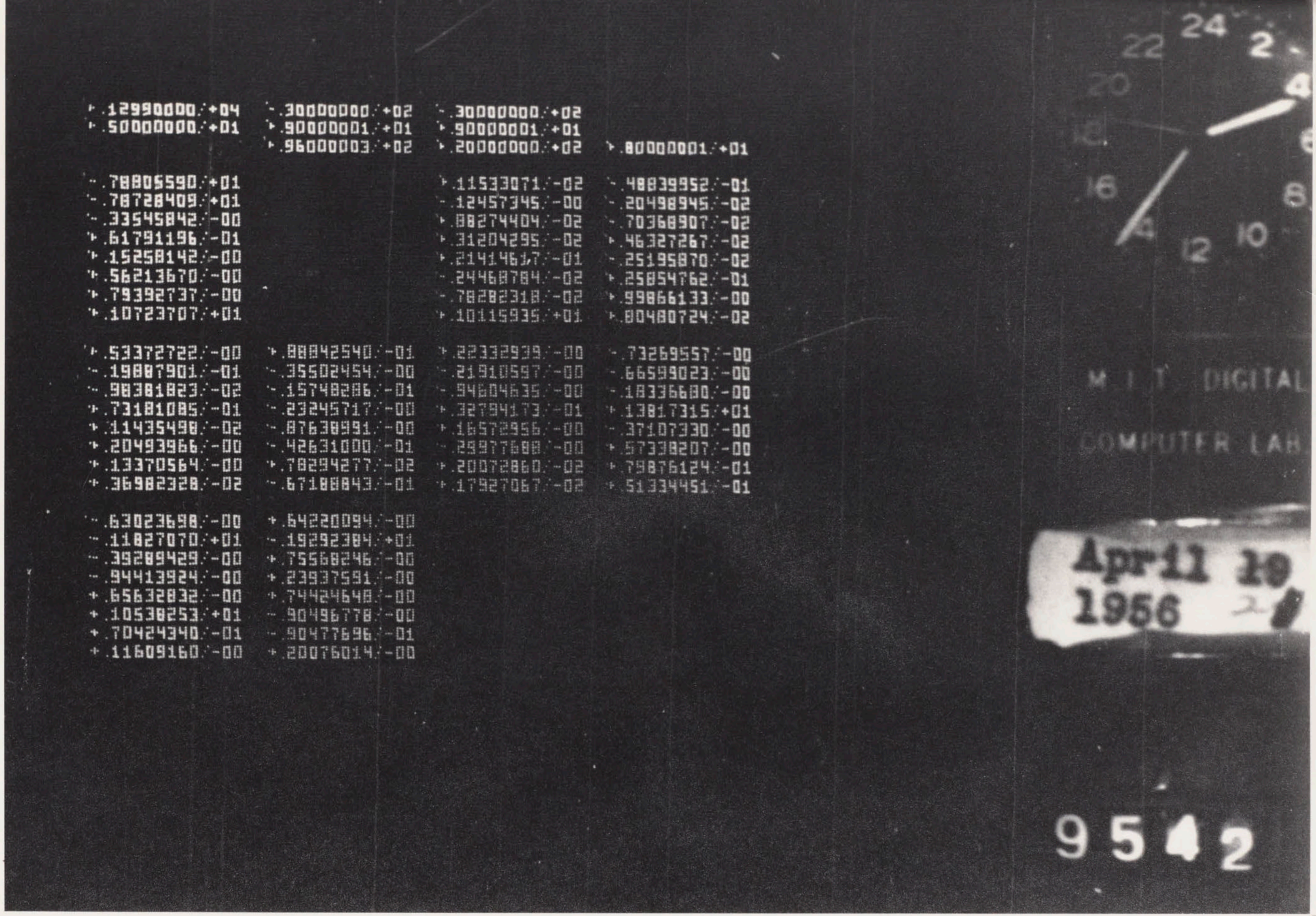

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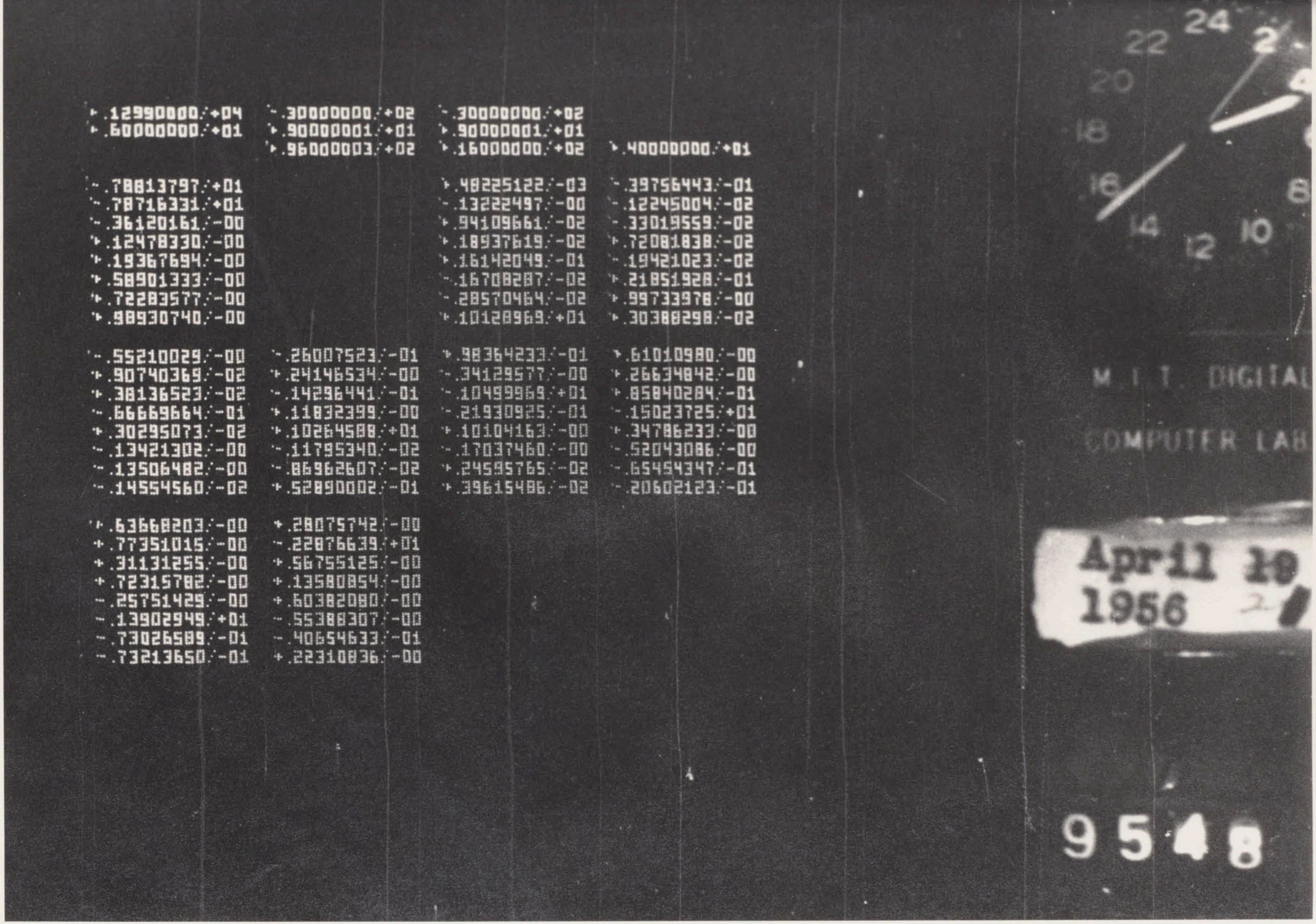

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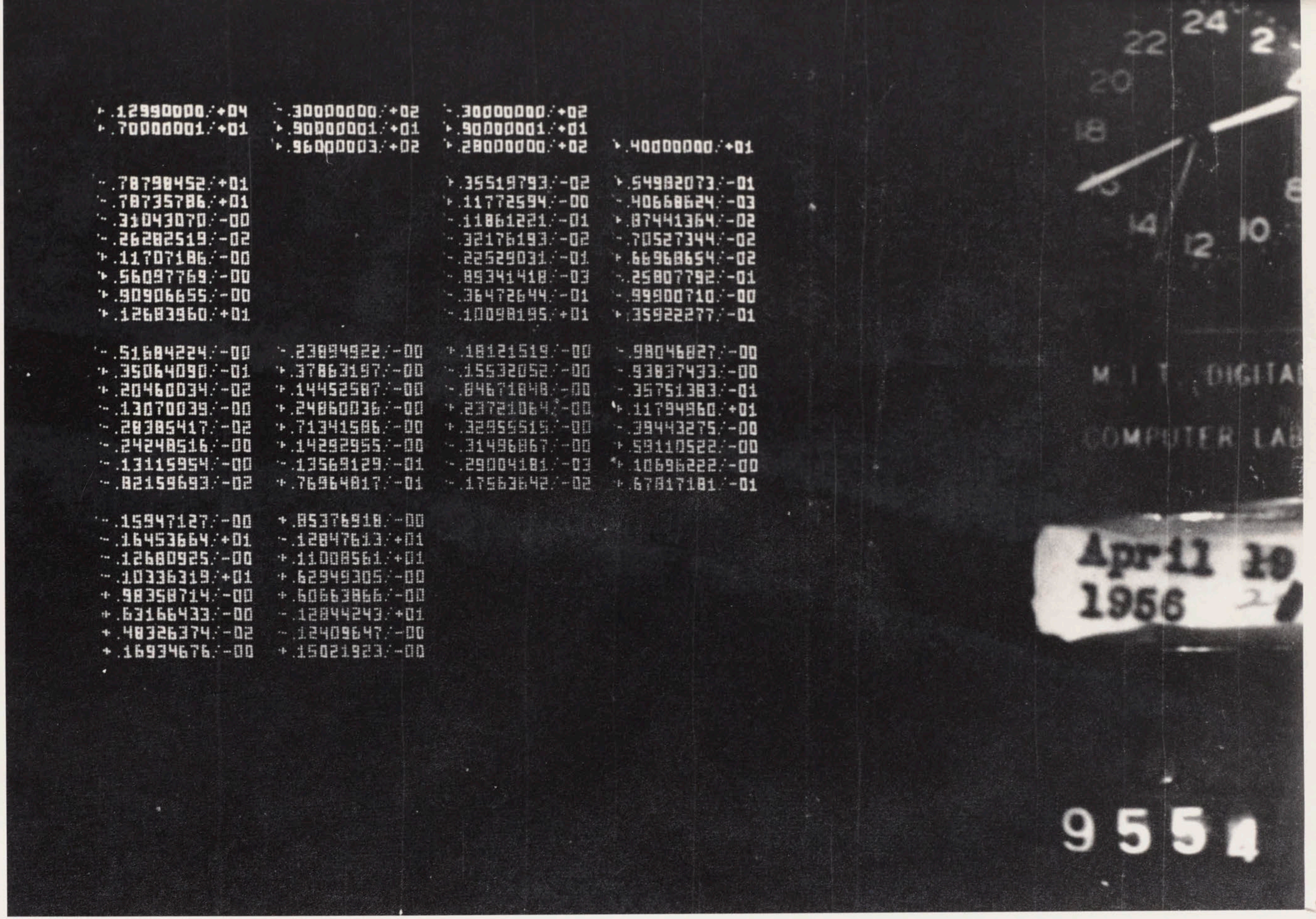

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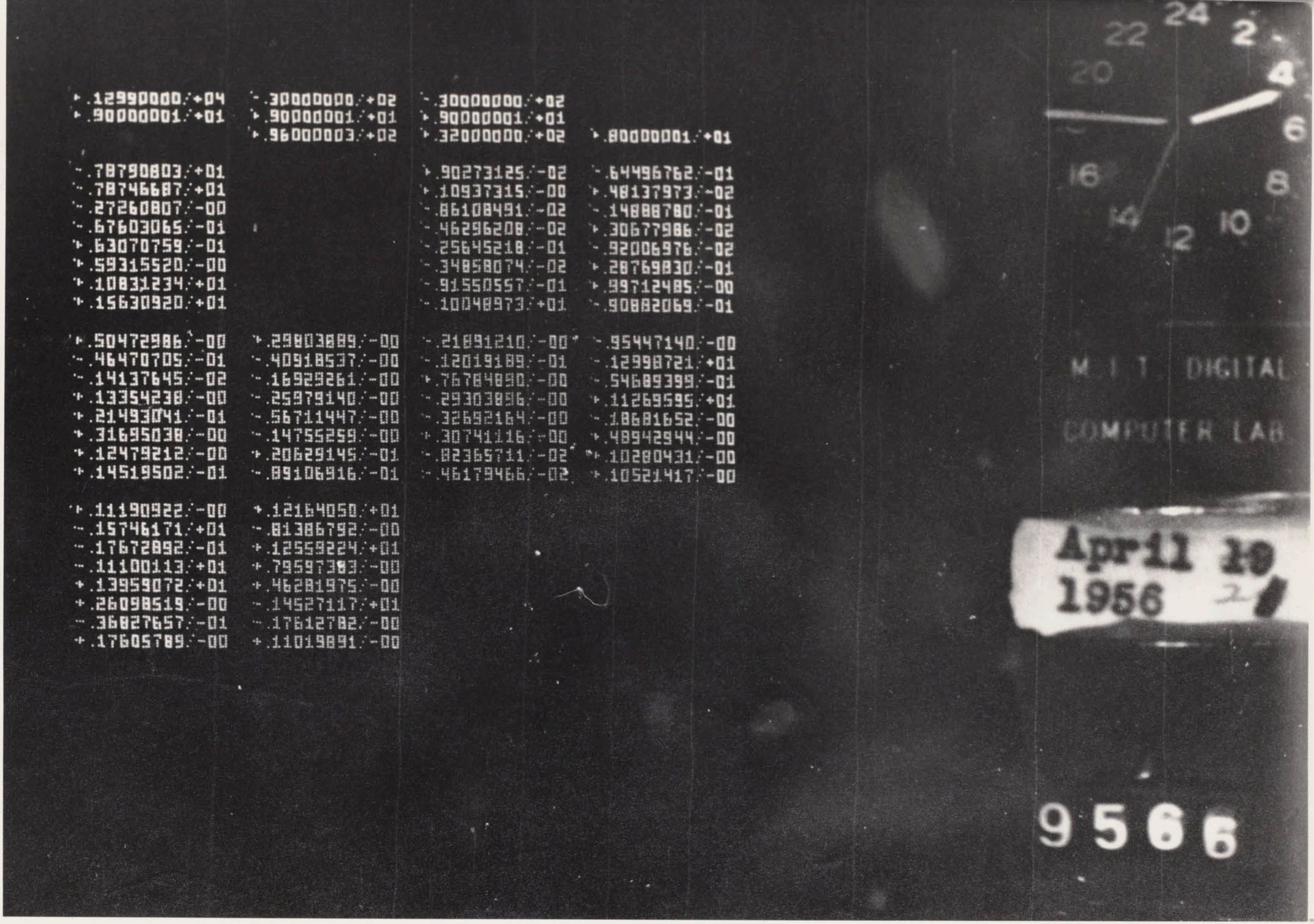

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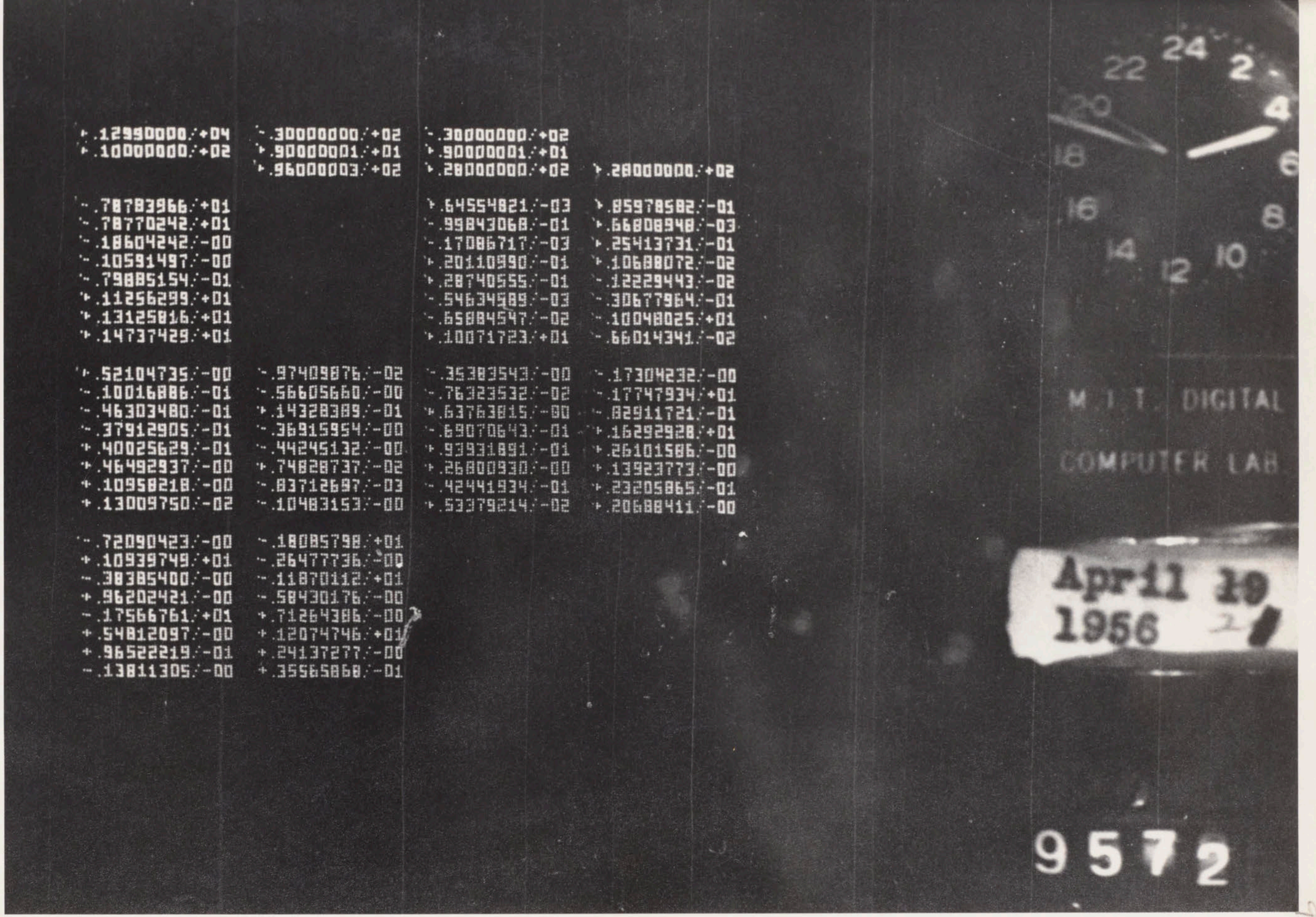

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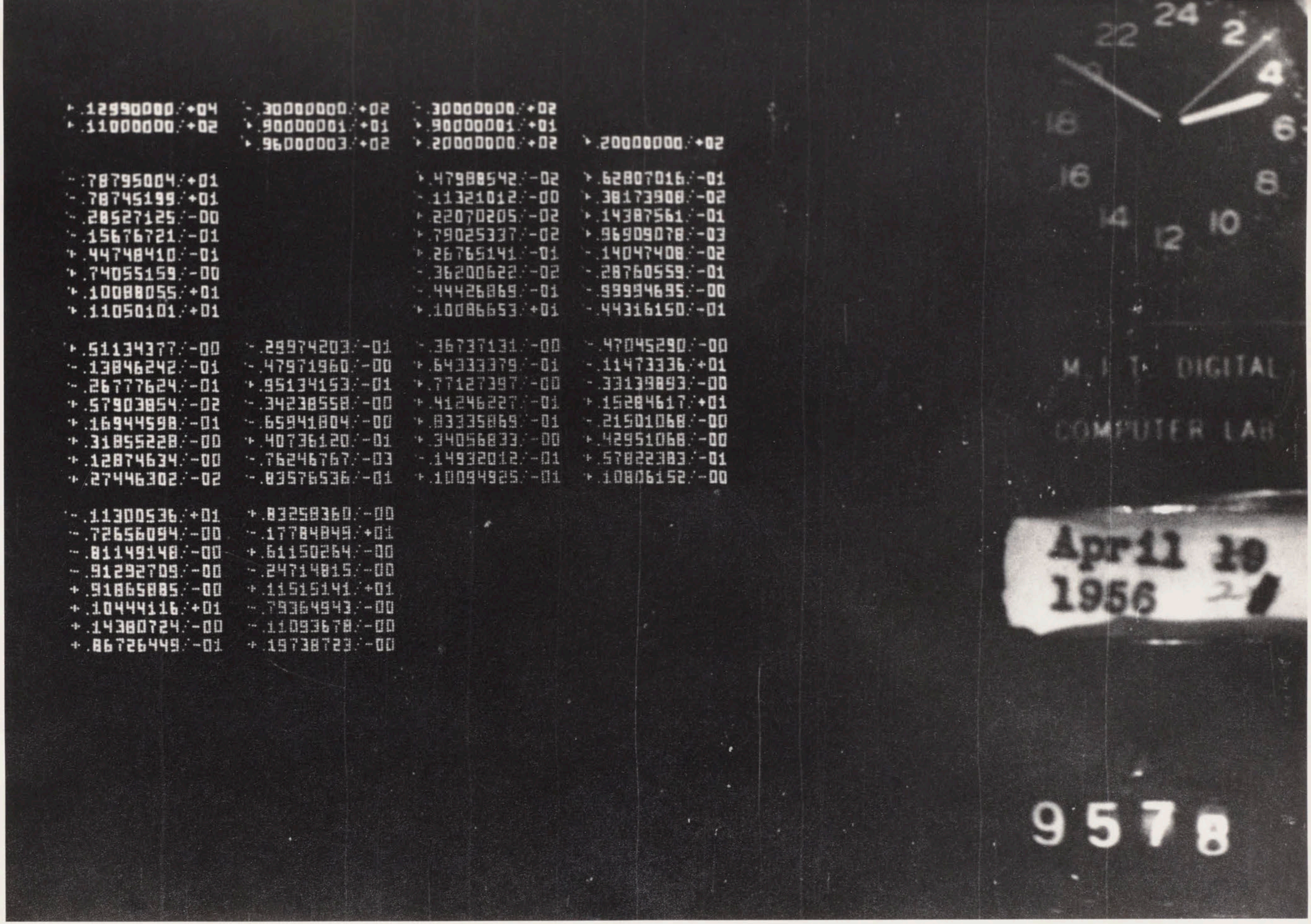

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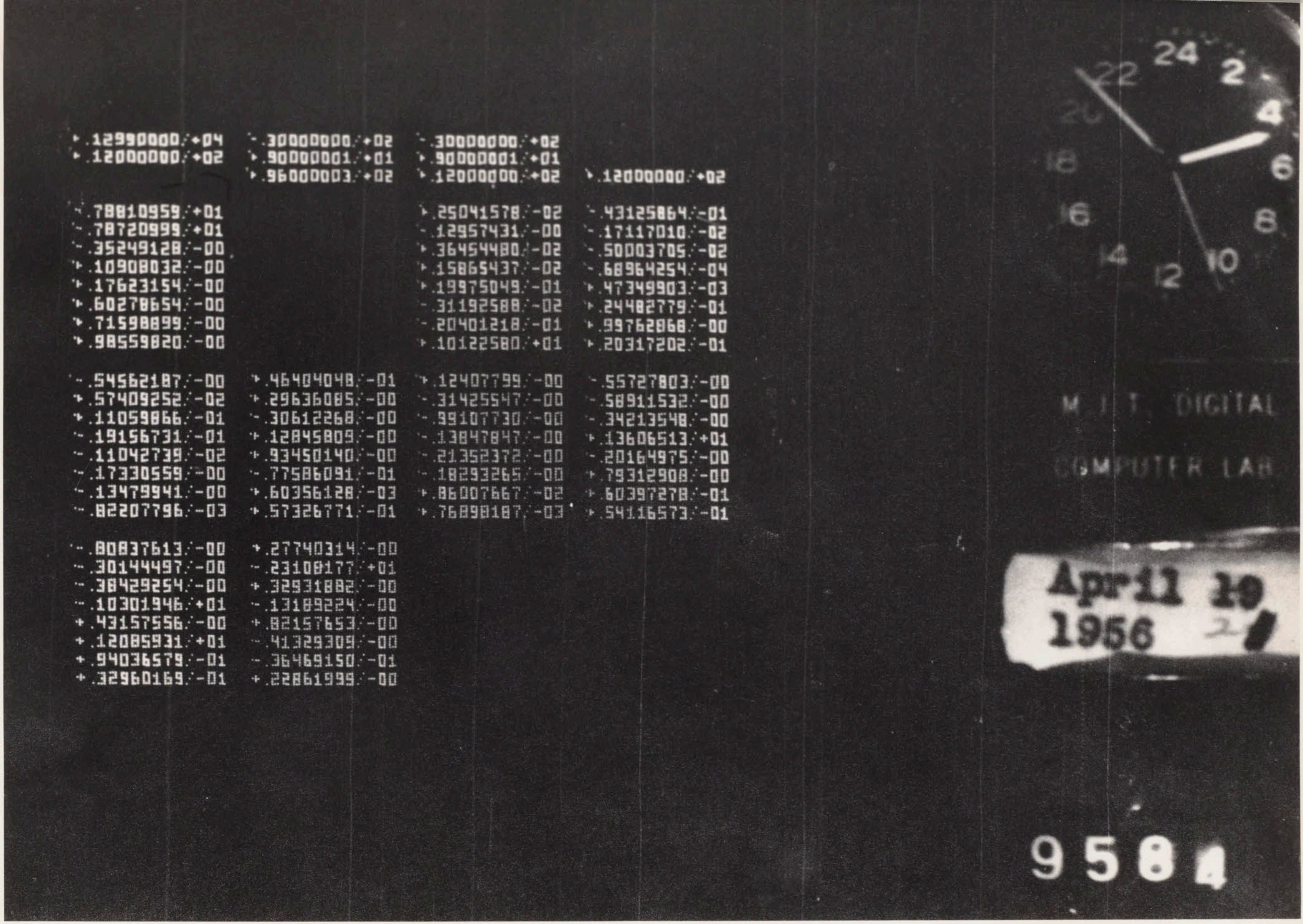

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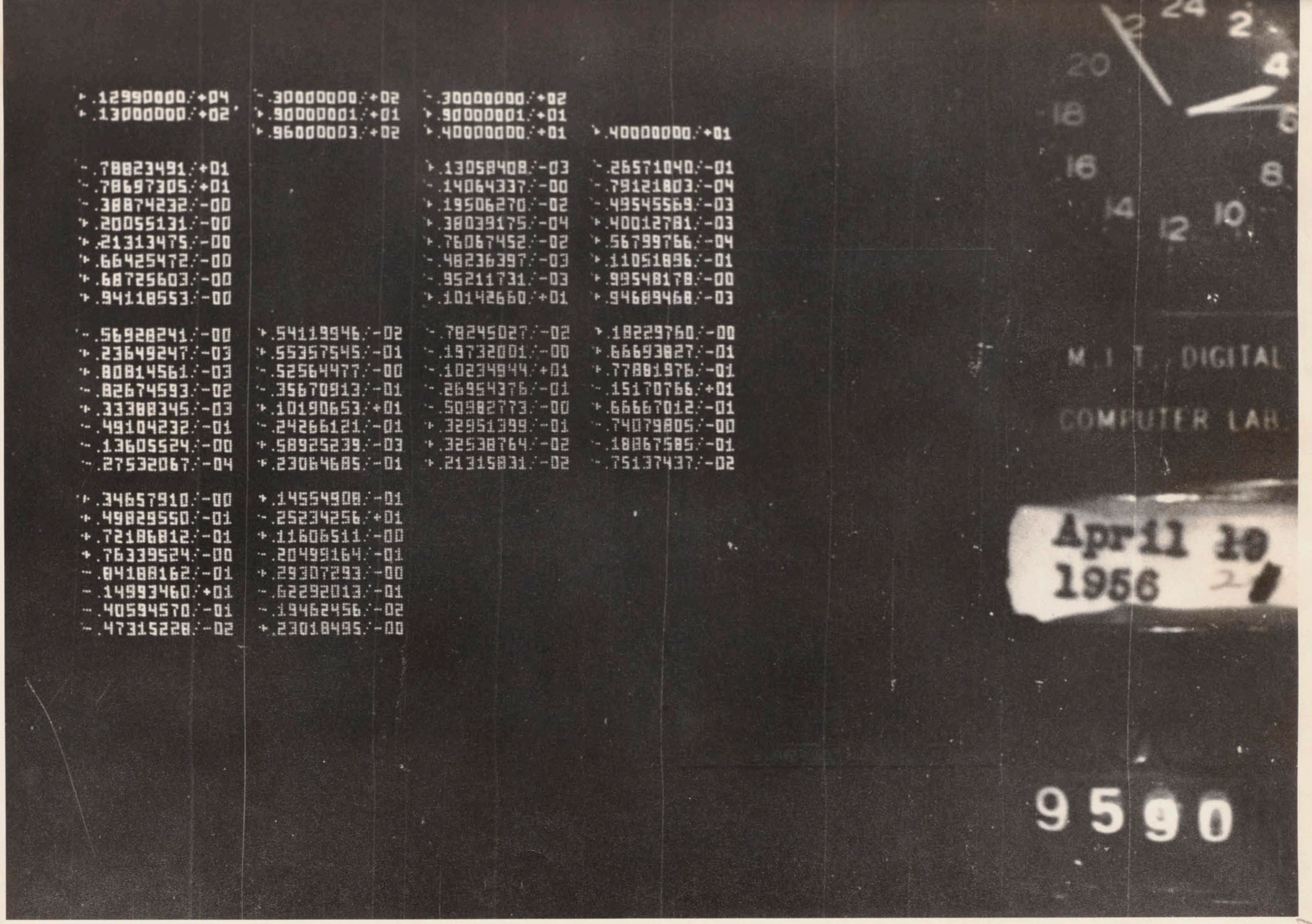

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